MATHEMATICAL MODELING OF PRODUCE WASHING IN AN INDUSTRIAL-SCALE FLUME WASHER

By

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ABSTRACT OF THE THESIS

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In America, fresh fruits and vegetables play an important role in enhancing people's health and wellbeing (FDA, 1998). However, the cross-contamination in a sanitizing chlorine washing system is considered as a potential area of risk, where the contaminated and non-contaminated produce are being washed together in the washer (Munther et al., 2015). Therefore, cross contamination of fresh produce during washing should be regarded as a critical risk factor that can lead to foodborne disease outbreaks. In addition, fresh produce and fruits are heavily handled but undergo minimal processing before consumption. Therefore, it is necessary to develop an efficient and effective process on produce washing.

In this study, two factors aimed to reduce the microbial load on the produce were considered, which were shear stress and free chlorine. Although many of chemical treatments have very high efficiency in reducing microbial population in wash water, most of the chemical forces have limitation when it comes to the removal of bacteria

from produce surface (Gil et al., 2009). In the removal of pathogens from produce surface, shear stress serves as the mechanical force and chlorine serves as the chemical force. During the washing process, bacteria get detached from the produce surface and go into wash water. However, some of the bacteria in wash water might re-attach on to the produce surface. The aim of this study was to mathematically model the combined role of shear stress and free chlorine on microbial attachment and adhesion in an industrial scale flume washer.

COMSOL® Multiphysics was used to simulate the washing of spherical produce in an industrial-scale flume washer. The first step was to examine how the relative horizontal positioning of two spherical produce impacted their exposure to shear stress caused by the flow in flume washer. Two spheres, 1.2 inches in diameter, were placed one behind another in a flume to represent spherical produce. The distance between the two spheres was varied. The correlation between the surface shear stress and the distance between two spheres was investigated. The simulated shear stress values were used in a mathematical model that simulated bacteria adhesion. A set of ordinary differential equations (ODEs) that described the ligand-receptor binding of bacteria and produce surface was used to quantify the number of bacteria detached and attached on the produce surface as a function of time. The shear stress values from prior simulation and chlorine sanitizer concentration were introduced to the ODEs to investigate their impact on the detachment and attachment of bacteria in this industrial-scale flume washer.

This study also effectively simulated the transport of free chlorine in a flume washer when chlorine was injected at selected locations. A chlorine dynamics model was used to calculate the distribution of chlorine in a flume washer.

The results showed that there was no significant change in the shear stress experienced by the sphere upstream when the distance between the two spheres was changed. The downstream sphere experienced variable shear stress, with shear stress reaching steady maximum value of 275 mPa when distance between the two spheres was no less than four times as their diameter. The ODEs approximated the number of bacteria on produce surface and in wash water under different shear stress values. Low main-flow velocity with higher injection velocity gave more uniform distribution of free chlorine. The results of this study will provide guidelines for designing produce washing equipment and the flow conditions used in produce washing.

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CHAPTER 1. INTRODUCTION

1.1. Background

Adequate consumption of fresh produce is a significant component of a healthy diet and serves as an effective approach in preventing many chronic diseases (WHO, 2016). However, recent outbreaks of food-borne illnesses happened with fresh produce negatively impact people's willingness to purchase and consume fresh-cut produce (Luo et al., 2018). The reason why pathogenic bacteria are often associated with fresh-cut produce is because processing water is an ideal catalyzer for the potential cross contamination of bacteria pathogens during fresh-cut produce washing (Luo et al., 2012). Therefore, a better understanding of the produce washing process is very important for optimizing the washing conditions and for designing new washing system so as to reduce the outbreaks of food-borne illness associated with fresh produce.

1.2. Produce washing by using sanitizer

Fresh produce washing can be conducted by various kinds of washing systems and using different washing fluids. Flume washer systems are commonly used in industrial produce washing process (see FIGURE 1). Flume washer is a open-channel washing system in which agitated turbulent flow is generated to remove dirt or bacteria on produce surface and a chemical sanitizer is injected to inactivate bacteria in wash water. This study investigated the produce washing process in an industrial-scale flume washer system. Chemical sanitizers are often used in commercial washing of fresh-cut produce in a flume washer in order to minimize the cross-contamination from the wash

water (Davidson at al., 2013). For example, chlorine and peroxyacetic acid (PAA) are often used as a produce washing sanitizer. The chlorine is recommended to use in the concentration of 25 ppm and the peroxyacetic acid (PAA) is used in 80 ppm (Lawton et al., 2015). The use of chlorine as a sanitizer in produce washing is regarded as the most effective when appropriate dose is added into the wash water (Gil et al., 2009). In the chlorine sanitizer, hypochlorous acid and hypochlorite can be maintained as the main chlorine species to serve as antimicrobial when pH ranges from 6 to 9 (Deborde, Marie, and Urs Von Gunten, 2008). Therefore, one of the critical factors to minimize the cross-contamination during produce washing is the addition of adequate amount of chlorine and its distribution in the washing system. It is necessary to investigate how much chlorine is needed to inactivate the bacteria in wash water and how fast the bacteria can be inactivated.

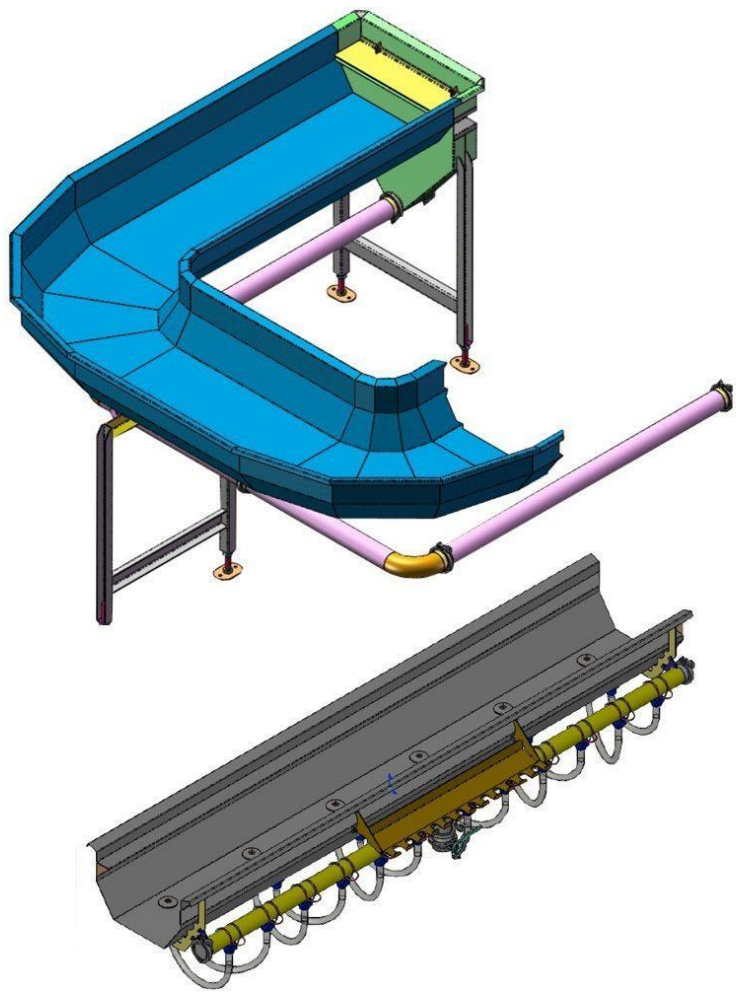


FIGURE 1 The 2400 Open Flume Systems from Heinzen® Manufacturing International. The top flume is the infeed section and the bottom flume is the washing system. Produce are transported by the top flume and are washed in the washing system on the bottom. (www.heinzen.com/processing-solutions/washing)

1.3. The role of shear force in produce washing

Besides the bacteria in wash water, there usually are certain amount of bacteria attached to the produce surface. A ligand-receptor binding model uses detachment constant and attachment constant to describe how bacteria detach and attach on the surface (Wang & Bryers, 1997). In this model, the detachment constant that is directly affected by the shear rate on the surface, which is regarded a critical factor in the removal of bacteria from the produce surface during produce washing. The shear force plays a

significant role in removing bacteria from produce surface compared to chemical sanitizer (Gil et al., 2009). Shear force was generated at the interface between water and produce surface due to flow. The shear rate values from 100 s^{-1} to 400 s^{-1} were used to detach bacteria from surface in Wang & Bryers 1997's study. Currently, it is almost impossible to measure the shear force on produce surface in an industrial flume washer. Therefore, it is necessary to calculate or estimate the shear stress distribution on a produce surface using mathematical simulations. Both the chemical force, which is caused by the chlorine sanitizer, and the mechanical force, which is due to shear stress or shear rate, was investigated to predict their combined role of controlling cross-contamination and bacterial load during produce washing in a flume washing system.

1.4. Mechanism of bacterial attachment: ligand-receptor binding

Ligand-receptor binding model had been used to describe the way bacteria in the wash water bind to produce surface during a washing process. Based on this specific binding mechanism, Wang and Bryers (1997) developed a mathematical model, which was then used to predict bacterial attachment and detachment during produce washing. Sufficient evidence suggests that specific molecules, receptors, on cells surface can bind to the complementary molecules, ligands, on target surface through a highly selective way (Ofek et al., 1978). The specific ligand-receptor binding describes the specific binding between receptor molecules on the cell and ligands associated with the target surface (Wang & Bryers, 1997). This specific ligand-receptor adhesion is one of the well-known binding mechanisms in bacterial infections and inflammations. Such specific

binding mechanism ensures the firm attachment to the target surface for bacteria (Wang & Bryers, 1997).

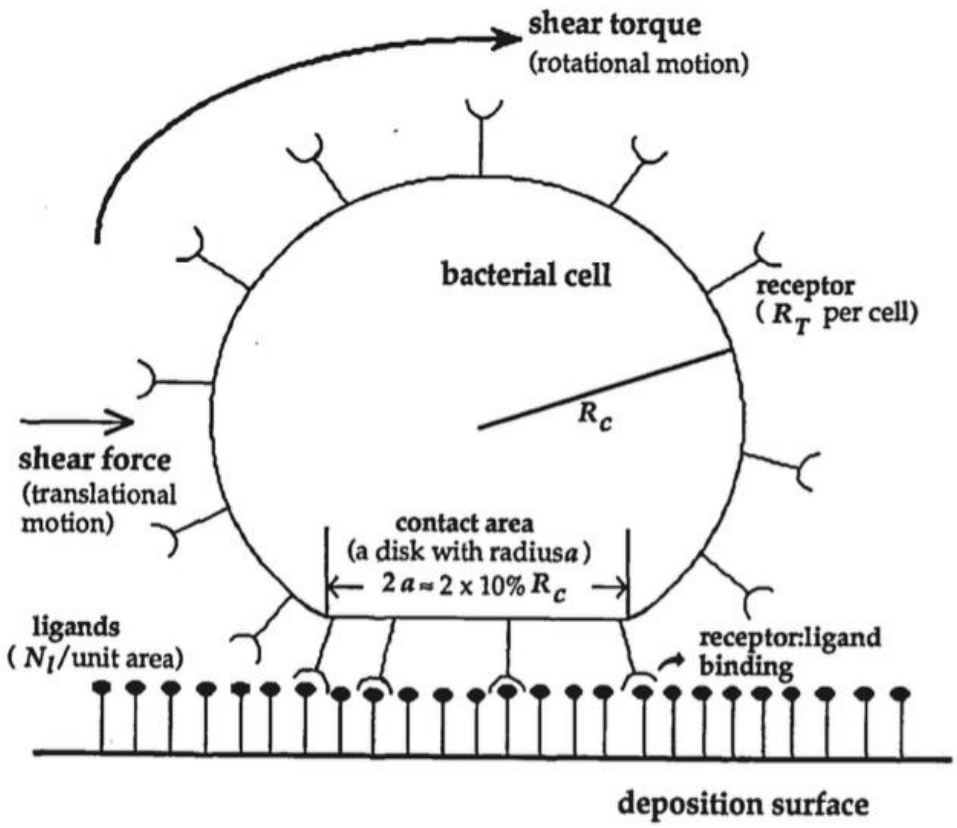


FIGURE 2 Pictorial representation of a bacterial cell-surface system in a uniform shear flow (Wang & Bryers, 1997). The bacterial cell is assumed to be spherical, while the disk-shaped contact area can be considered as a circle with radius a, which is 10% of the cell radius R_c according to Wang and Bryers. There are R_T of receptors per cell and N_l of ligands per unit area on the deposition surface.

1.5. Mathematical model of bacterial attachment and detachment

Based on the specific receptor-ligand binding, Wang & Bryers (1997) developed a dynamic model to describe bacterial cell adhesion in viscous shear flow. In this model, a set of non-linear ordinary differential equations (ODEs) were derived, which demonstrated the net accumulation of cell number on surface of ligand-coated surface, cell number and sanitizer concentration in the solution passing over the ligand-coated surface."

In the literature, the time rate of changes in surface cell number (B), wash water cell number (X), and the sanitizer concentration (C) can be given as follows (Wang & Bryers, 1997):

$$\frac{dB}{dt} = K_{adh}X - k_{det}B + \frac{\mu_{max}C}{(k_s+C)}B \qquad (1)$$

$$\frac{dX}{dt} = D(X_{in} - X) - K_{adh}X\frac{A}{V} + k_{det}B\frac{A}{V} \qquad (2)$$

$$\frac{dC}{dt} = D(C_{in} - C) - \frac{\mu_{max}CB}{(k_s+C)Y} \cdot \frac{A}{V} \qquad (3)$$

Where

B = number of cells attached to produce surface per unit area at time t (# of cells/cm^2)

X = number of cells suspended in wash water at time t (# of cells/cm^3)

X_{in} = inlet concentration of cells in wash water (# of cells/cm^3)

C = sanitizer concentration at time t (g/cm^3)

C_{in} = inlet sanitizer concentration (g/cm^3)

t = time (min)

D = dilution rate (min^{-1}) = flow rate/washer volume

k_{det} = detachment rate constant (min^{-1})

K_{adh} = overall adhesion rate constant (cm/min)

A = substratum area (cm^2)

V = reactor volume (cm^3)

Y = yield of attached cells

k_s = saturation coefficient (g cm^{-3})

μ_{max}= maximum specific growth rate of attached cell (min^{-1})

Since the growth rate of bacteria was ignored, which means the term $\mu_{max} = 0$, derivation of the ODEs can be described as follows (more explanations of the ODEs can be found in section 2.4.1):

According to mass balance of the bacterial cells and chlorine concentration (see FIGURE 3), three balances can be established:

<u>Mass balance of bacterial cells on produce surface</u>:

(number of bacteria on produce surface per unit of area at time t) = (number of bacteria attached onto produce surface per unit of area) – (number of bacteria detached from produce surface per unit of area)

<u>Mass balance of bacterial cells in wash water</u>:

(number of cells suspended in wash water per unit of volume at time t) = (dilution effect by the wash water) – (number of cells attached onto produce surface per unit of volume) + (number of cells detached from produce surface per unit of volume)

Mass balance of chlorine in wash water:

(sanitizer concentration at time t) = (dilution effect by the wash water). The effect of chlorine natural decay and depletion by organic matter will be considered in the following section 2.1.

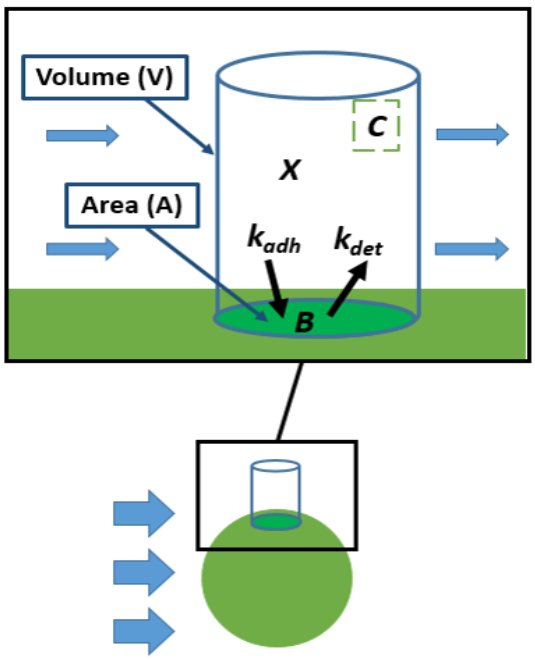


FIGURE 3 Mass balance of bacteria cells and chlorine in the detachment and attachment model

Using the mathematical symbols, the mass balance can be derived as follows:

$$\frac{dB}{dt} = K_{adh}X - k_{det}B \quad (4)$$

$$\frac{dX}{dt} = D(X_{in} - X) - K_{adh}X\frac{A}{V} + k_{det}B\frac{A}{V} \quad (5) = (2)$$

$$\frac{dC}{dt} = D(C_{in} - C) \quad (6)$$

Where

$K_{adh}X$ = Number of bacteria attached onto produce surface per unit of area

$k_{det}B$ = number of bacteria detached from produce surface per unit of area

$D(X_{in} - X)$ = dilution effect on cells number in wash water

$K_{adh}X\frac{A}{V}$ = number of cells attached onto produce surface per unit of volume

$k_{det}B\frac{A}{V}$ = number of cells detached from produce surface per unit of volume

$D(C_{in} - C)$ = dilution effect on sanitizer concentration in wash water

Based on the ODEs (4), (5) and (6), the number of bacteria attaching on the surface per minute is governed by two factors (i) the number of bacteria cells already attached on the surface (X) and (ii) the number of cells in the wash water (B). Therefore, if the adhesion rate constant (K_{adh}) remains unchanged, the number of bacteria cells on the surface is significantly affected by the detachment constant (k_{det}), which changes according to the shear force applied on the surface. As the bacterial cells are detached

from the produce surface, they are inactivated by the added chlorine sanitizer. Bacteria concentration also reduces due to dilution effect of the flow and the specific adhesion of bacterial cells that binds them onto the surface. Detached bacterial cells go into the wash water, which increases the bacteria concentration in the water. Lastly, the sanitizer concentration is affected by the dilution factor and natural decay of chlorine described in the following section. The depletion of chlorine by organic matter also plays a significant role in distribution of the chlorine sanitizer concentration in the washer system.

1.6. Rationale

Numerical simulations of the inactivation of bacteria during produce washing in the industry are rarely conducted because simulations of produce washing requires a huge amount of cost in simulation software and hiring numerical simulation experts. The combined role of shear force and chemical sanitizer should be investigated to ensure the effectiveness of the washing system. Therefore, it is beneficial to develop an approach to quantify the effectiveness of produce washing for the processing industry. Taking both surface shear force and chlorine sanitizing effect into considerations, this study aimed at quantifying the number of bacteria removed and inactivated during produce washing, which can provide a guideline to the produce washing industry on the validation of washing effectiveness.

1.7. Objectives

The overall goal of this study was to provide the produce washing industry with a guideline, based on which the inactivation of bacteria in produce washing and the level of chlorine used can be numerically simulated and thus quantified. This can be used to validate the effectiveness of produce washing process in an industry setting.

The first objective was to numerically simulate the cross-contamination and inactivation of bacteria during the produce washing process in an industrial-scale flume washer system. In this part, the effect of the distance between each individual spherical produce on the surface shear force was studied. The surface shear force was calculated and was considered together with chlorine sanitizer to predict the removal and inactivation of bacteria during washing process.

Another objective was to investigate the distribution of chlorine sanitizer inside a flume washer under different flow conditions. The chlorine was injected from the bottom of the flume. The goal was to provide numerical results on how flow conditions affects the distribution of sanitizer in a flume washer.

The observations and methods of this study can be used to predict the amount of shear stress on each produce at given condition (flow rate and number of produce in the tank). This study can also provide information, such as at what produce feeding rate or wash water flow rate, produces can be washed properly.

CHAPTER 2. MATHEMATICAL MODELING

Based on the design of an industrial-scale flume washer, mathematical modeling and numerical simulation of produce washing process were conducted in this study. Using COMSOL® Multiphysics, the amount of shear stress applied on the produce surface under controlled flow condition was calculated. In the simulations, only spherical geometry was investigated. The shear stress calculated from the simulations was used to obtain a rate constant, which described how fast the surface bacteria were being detached from the produce surface. The detachment rate constant was then applied to a set of ordinary differential equations (ODEs), which described the situation when there were multiple spherical produce suspended in the wash water. The removal of surface bacteria and the bacterial load in wash water were predicted by the ODEs.

This research used numerical simulation tool COMSOL® Multiphysics to solve the fluid flow in a flume washer so as to obtain a key physical parameter (surface shear rate η), which was then converted to detachment rate constant (k_{det}). The ordinary differential equations (ODEs) were derived that characterized the contribution of both chemical force and mechanical force in controlling the bacterial level in a wash system. Then the relationship between detachment rate constant (k_{det}) and shear stress was derived. These two segments were connected by the detachment rate constant (k_{det}). The numerical model predicted three critical values in produce washing, which were surface bacterial load (B), wash water bacterial load (X), and sanitizer concentration (C).

2.1. Numerical simulation of produce washing

Besides the shear force that contributes to the removal of bacterial cells from the produce surface, sanitizer like chlorine also plays a very significant role in controlling the bacteria concentration in wash water. A mathematical model for pathogen cross-contamination dynamics during produce washing derived by Munther et al. (2015) can quantify the inactivation of the bacterial cells in the wash water by chlorine sanitizer. In this model, chlorine concentration also decreased due to natural decay of chlorine and depletion by organic matter in wash water (Munther et al., 2015). However, they did not consider the situation when water was being recycled nor being filtered. In response to that, this study included the recirculation of the washing water into the model. Wash water was not filtered but only recycled in this model. As the wash water was recycled during the washing process, the bacteria load in wash water existing the system equaled the bacteria load entering the system from the inlet. Based on that, the terms X_{in} should equal to X meaning the term $D(X_{in} - X)$ in equation (5) should be zero.

$$\frac{dB}{dt} = K_{adh}X - k_{det}B \qquad (4)$$

$$\frac{dX}{dt} = D(X_{in} - X) - K_{adh}X\frac{A}{V} + k_{det}B\frac{A}{V} \qquad (5) = (2)$$

$$\frac{dC}{dt} = D(C_{in} - C) \qquad (6)$$

When considering wash water recirculation, chlorine natural decay, and chlorine depletion by organic matter, equations (4), (5), and (6) can be modified to the following equations:

$$\frac{dB}{dt} = K_{adh}X - k_{det}B \qquad (7) = (4)$$

$$\frac{dX}{dt} = k_{det}B\frac{A}{V} - K_{adh}X\frac{A}{V} - \alpha XC \qquad (8)$$

$$\frac{dC}{dt} = D(C_{in} - C) - \lambda C - \beta OC \qquad (9)$$

Where

α = inactivation rate of bacterial cells by sanitizer (L/(mg min))

β = depletion rate of sanitizer by organic matter (L/(mg min))

λ = natural decay rate of chlorine (min-1)

O = amount of organic matter (mg/L)

During the produce washing process, the amount of organic matter keeps increasing when more and more produce are added into the washing system (Luo et al., 2012). Therefore, in the mathematical model the amount of organic matter (O) was set to increase with time in the rate of k0 (Munther et al., 2015):

$$O = k_0 t \qquad (10)$$

The solution to the above ordinary deferential equations (ODEs) should enable numerical simulation of the produce washing process by predicting both the surface bacterial number (B) and wash water bacterial level (X) while taking the mechanical force (shear rate or kdet) and chemical force (C and α) into consideration. This set of ODEs was solved by MATLAB® using Runge-Kutta fourth-order method and used to analyze the produce washing process in an industrial-scale flume washer. The shear rate value obtained from simulations in COMSOL® Multiphysics needed to be converted to

detachment rate constant (k_{det}) in equations (7) and (8), which quantified the number of bacteria on produce surface and in wash water. Therefore, numerical simulation of the produce washing in the flume washing system was achieved. The logic flow of this study is shown in FIGURE 4.

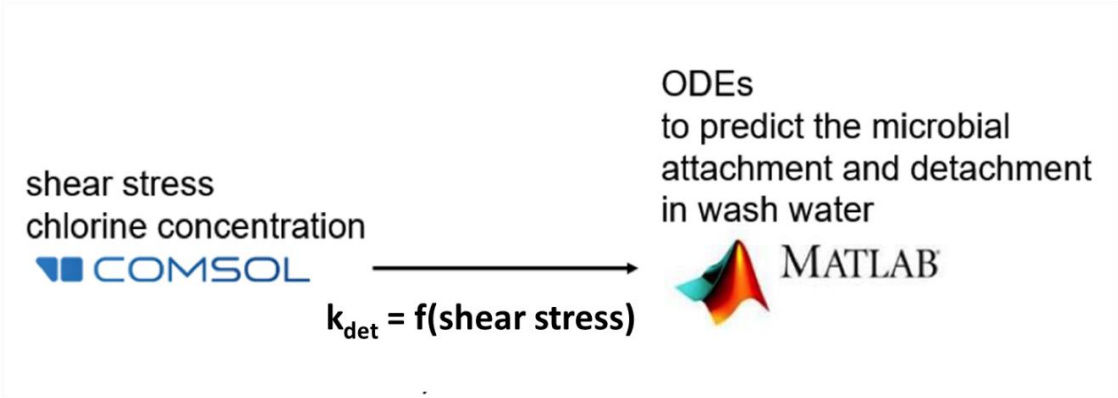


FIGURE 4 The logic flow of this study.

2.2. Relationship between shear force and detachment rate constant

One key step of connecting numerical simulation of fluid flow in the flume washer to the ODEs describing attachment-detachment of bacteria was to establish the relationship between shear force and detachment rate constant (k_{det}). This is because the detachment rate constant is a critical parameter that appears in the ODEs which governs the number of bacterial cells on the surface and in the flow domain. The shear force was numerically calculated on the spherical produce surface using COMSOL® Multiphysics. The derivation of the relationship between k_{det} and shear force was obtained from related literatures (Bell, 1978; Hammer & Lauffenburger, 1989; Lawrence & Springer, 1991;

Schlichting, 2017; Wang & Bryers, 1997). The equations used in the derivation are as follows:

$$k_{det} = k_{det}^{0} \exp\left(\frac{\gamma F_b}{k_b T}\right) \quad (11)$$

Where

k_{det}^{0}= base value of detachment constant (min^{-1})

γ = bond length (cm)

k_b = Boltzmann constant (erg/K)

T = temperature (K)

F_b = force acting on each bond (N)

$$F_t = N_b A_c F_b = 6\pi\mu(R_c)^{2\eta}(Root) \quad (12)$$

$$F_b = \frac{6\pi R_c^2 \eta(Root)}{N_b A_c} \quad (13)$$

Where

R_c = radius of the cells (cm)

μ = fluid viscosity (mPa s)

η = shear rate (s^{-1})

A_c = contact area size (cm^2)

N_b = bond density (# of bonds / cm^2)

Root = a unit-less constant shown in TABLE 1 (Wang & Bryers, 1997)

$$F_b = \frac{6(\mathrm{Root})\eta}{N_b} \tag{14}$$

$$N_b = \frac{k_f R_T (\frac{A_c}{S_{area}}) N_l}{k_f R_T \left(\frac{A_c}{S_{area}}\right) + k_{det}^0} \tag{15}$$

$$K_{adh} = k_f R_T \frac{V}{A} = k_f R_T l \tag{16}$$

Where

R_T = receptor number

N_l = ligand density (# of ligand / cm^2)

S_{area} = surface area of one cell (cm^2)

k_f = specific rate constant (per cell min^{-1} # of $receptor^{-1}$)

l = boundary layer thickness (cm) (shown in FIGURE 5)

K_{adh} = adhesion rate constant (cm/min)

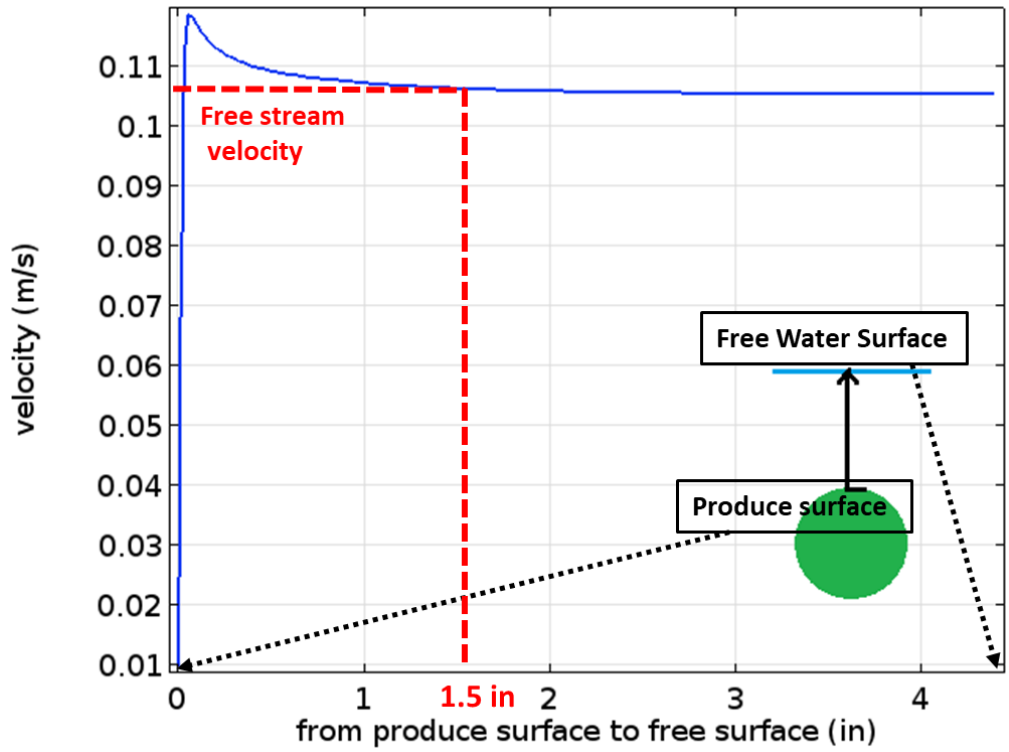


FIGURE 5 Boundary Layer Thickness around the spherical produce in the flow. The boundary layer thickness equals to the distance through the boundary layer from the surface to the point where the flow velocity reached 99% of the 'free stream velocity' (Schlichting, 2017). According to this graph, the boundary layer thickness is about 1.5 inches = 3.81 cm. The direction of the velocity was from left to right.

Table 1 gives the values of all the parameters described above. According to Table 1 and equations (11), (12), (13), (14), (15), and (16), derivation of equation (17) can be carried out and the relationship between shear rate (η) and detachment rate constant (k_{det}) shown as follow:

$$k_{det} = 0.007\exp(0.0179\eta) \qquad (17)$$

Using equation (17), the shear rate value obtained from COMSOL® Multiphysics could be converted into the detachment rate constant, which measured the strength of flow shear force on removal of bacterial cells on a spherical produce surface during

washing. According to equation (17) when the shear force increases, the detachment rate constant increases because higher the shear force or shear rate, faster the bacterial cells get detached from the surface.

TABLE 1 Parameter values used in the derivation

Parameter	Definition	Estimated value	References
R_T	Receptor number	10^3	(Hammer & Lauffenburger, 1989)
N_l	Ligand density	5^{11} cm^{-2}	(Hammer & Lauffenburger, 1989)
$\mathbf{k^0_{det}}$	Base value of detachment constant	0.0070 min^{-1}	(Wang & Bryers, 1997)
$\boldsymbol{\gamma}$	Characteristic bond length	5^{-11} cm	(Bell, 1978)
k_b	Boltzmann constant	1.38^{-16} erg/K	_
T	Temperature	293.15 K	_
R_c	Radius of the cells	10^{-6} cm	(Wang & Bryers, 1997)
$\boldsymbol{\mu}$	Fluid viscosity	0.01 g/(cm s)	(Lawrence & Springer, 1991)
Root	Constant	55.01	(Wang & Bryers, 1997)
K_{adh}	Adhesion rate constant	0.01 cm/min	(Wang & Bryers, 1997)
$\mathbf{l}$	Boundary layer thickness	3.81 cm	_

2.3. Flow past through two spherical produce in the industrial-scale flume washer

This segment investigated the situation where only 2 spherical produce were placed nearly in the center of the flow domain and being washed in the flume washer. This part of the study focused on how positioning of the two spherical produce, one behind the other, affected the shear force on their surfaces and therefore the detachment rate constant values on their surfaces. To investigate the impact of positioning of different produce on the surface shear force, the simulations were carried out and the distance between the spheres was increased as integral multiple of the sphere diameter (1.2 inches). 1.2 inches close to the diameter of typical small spherical produce such as brussel sprouts. The results of this study should reveal how the shear force on the produce surface is influenced by the presence of other produce near it.

This segment also simulated the scenario where multiple produce (more than 2 spheres) were placed one after another and filled up the entire layer close to the free water surface in the flume washer. The produce quantity should be packed to maximize the washing efficiency and the produce to wash fluid ratio should be as high as possible. In other words, the distance between consecutive produce was minimized.

2.3.1. Geometry

Geometry of a flume washer from Heinzen® Manufacturing International is shown in FIGURE 6. Based on actual industrial design, this geometry was simplified so the fluid flow problem could be solved using COMSOL® Multiphysics. The dimensions are shown in FIGURE 7. In the study of the impact of distance on surface shear force,

two spheres were placed inside the flume to represent spherical produce. The diameter of each sphere was 1.2 inches. Free surface boundary condition shown in Figure 8 means no shear force on the surface. Inlet uniform flow velocity was set as 0.1 m/s and the outlet pressure was 0 gage pressure.

FIGURE 6 Industrial-scale flume washer from Heinzen® Manufacturing International

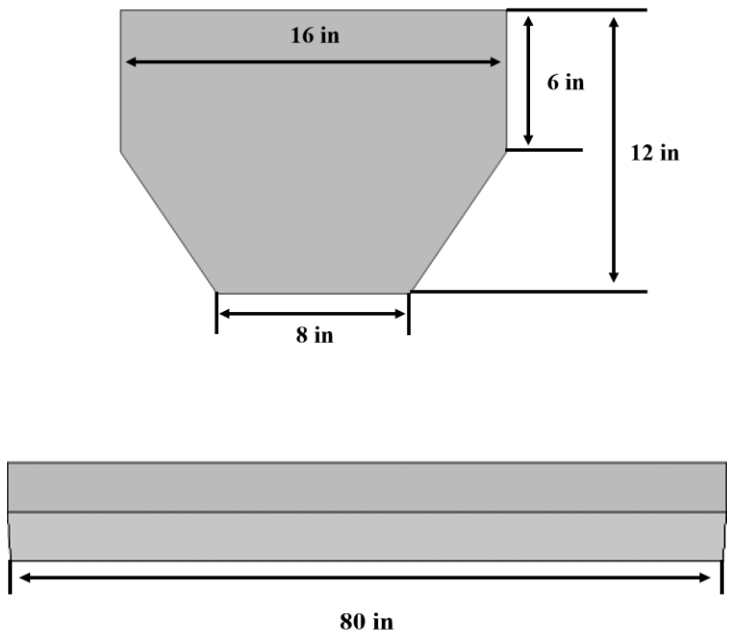


FIGURE 7 Geometry and dimensions of the flume washer. Cross-sectional view is the on the left and side view is on the right.

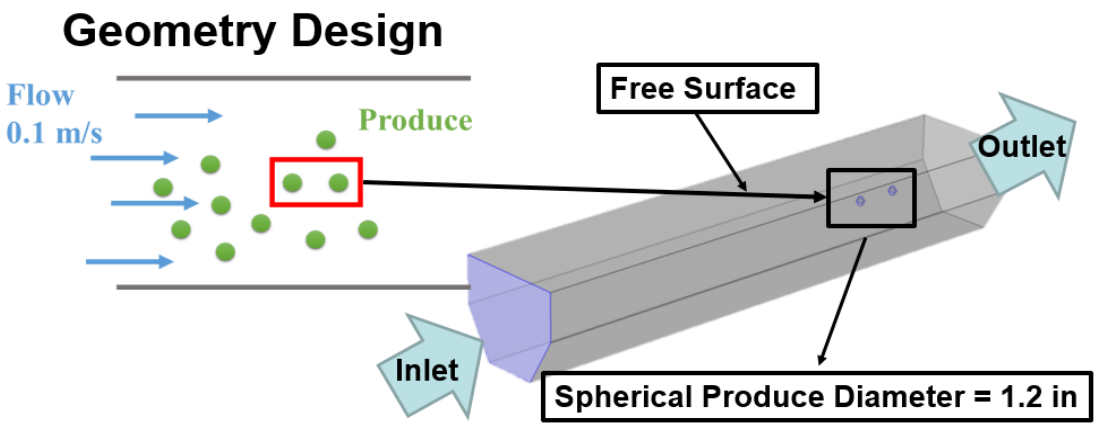


FIGURE 8 Geometry design used in simulations.

In the study that investigated the impact of distance between two consecutive spherical produce on surface shear force, only two spheres were placed in the flume washer as shown in FIGURE 8. If the spheres were too close to each other, they could influence each other in terms of the shear force on their surface. The goal of this study was to find out the minimum distance between the spheres so as not to affect shear force experienced by each sphere during the washing process.

2.3.2. Boundary condition and physics model in turbulent flow system

To ensure the flow velocity used in this study larger than the critical velocity of turbulent flow, the Reynolds number was calculated in accordance with the dimension of the flume washer and compared with the critical Reynolds number, which equals to 2900, for turbulent flow (Schlichting, 2017). The Reynolds number was calculated as follows (Reynolds, 1883):

Reynolds number = $\rho \upsilon d_h / \mu$ = 49700 > 2900 (critical Reynolds number)

Where,

ρ = density of water = 1000 kg/m^3

υ = flow velocity = 0.1 m/s

μ = viscosity of water = 0.001 Pa s

d_h = hydraulic radius = 4A (cross-sectional area)/ p (wetted perimeter) = 0.497 m

Wetted perimeter is the perimeter of the cross-sectional area that directly contacts with water (Schlichting, 2017). The critical Reynolds number is the lower limit for a flow to be a turbulent flow. When calculating the Reynolds number of flow in the flume, the viscosity and density of the wash water that contained chlorine sanitizer were assumed as the same as pure water.

2.3.3. Numerical Algorithm and Simulation

COMSOL® Multiphysics utilizes finite element method to solve problems. The software divides the entire domain into many small domains called as elements and solves the governing conservation equation in each of these elements. The software then combines the solutions from all the small elements all together, which is the solution for the whole domain. The main governing equation in this model, which is called the Reynolds-averaged Navier-Stokes (RANS) equation (18), was solved in COMSOL® Multiphysics during the simulations. Equation (19) called continuity equation was also solved together with RANS equation (18). The Navier-Stokes equation (18) represents the conservation of momentum and continuity equation represents the conservation of mass (COMSOL® Multiphysics Cyclopedia, 2015):

$$\rho(\mathrm{U}\cdot\nabla\mathrm{U}) + \nabla\cdot\left(\mu_{\mathrm{T}}(\nabla\mathrm{U} + (\nabla\mathrm{U})^{\mathrm{T}}) - \frac{2}{3}\mu_{\mathrm{T}}(\nabla\cdot\mathrm{U})\mathrm{I}\right)$$

$$= -\nabla\mathrm{P} + \nabla\cdot\left(\mu(\nabla\mathrm{U} + (\nabla\mathrm{U})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathrm{U})\mathrm{I}\right) + \mathrm{F} \qquad (18)$$

$$\frac{\partial\,\rho}{\partial t} + \nabla\cdot\,\rho\,\mathrm{U}=0 \qquad (19)$$

Where U is the fluid velocity, P is the fluid pressure, ρ is the fluid density, and μ is the fluid dynamic viscosity. The term '$\rho(\mathrm{U}\cdot\nabla\mathrm{U}) + \nabla\cdot\left(\mu_{\mathrm{T}}(\nabla\mathrm{U} + (\nabla\mathrm{U})^{\mathrm{T}}) - \frac{2}{3}\mu_{\mathrm{T}}(\nabla\cdot\mathrm{U})\mathrm{I}\right)$' measures the inertial force, '$-\nabla\mathrm{P}$' for pressure force, '$\nabla\cdot\left(\mu(\nabla\mathrm{U} + (\nabla\mathrm{U})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathrm{U})\mathrm{I}\right)$' for viscous force, and 'F' for the external force applied to the fluid (Batchelor, 1967).

With the RANS equation (18) and the continuity equation (19), COMSOL® Multiphysics solved the equations in each small element, which is also called mesh shown in FIGURE 9, and then combined all the results in each element into the numerical results of the fluid dynamic simulations. The number of mesh was the highest on the sphere surface and gradually decreased away from the sphere surface. Therefore, the meshes were extremely fine on or near produce surface and were very coarse in the other area of the flume. The total number of these small elements in the 3D geometry was about 1322348. Typical solving time of the simulations was about 2 hours.

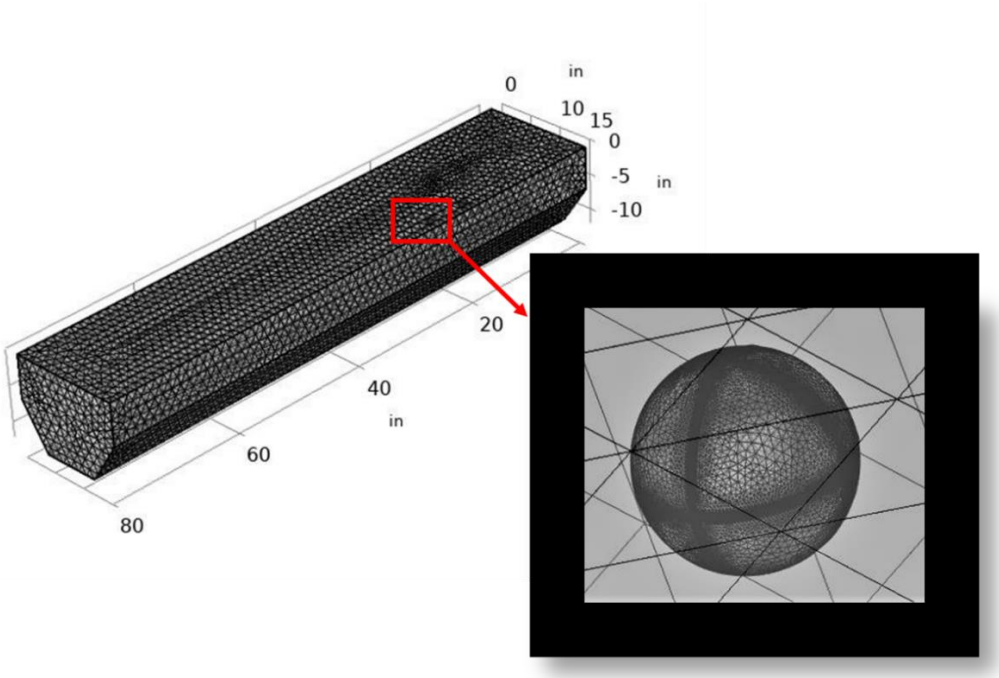


FIGURE 9 Mesh in the 3D geometry

In order to solve the governing equations, boundary conditions have to be applied which are shown in Table 2.

TABLE 2 Boundary conditions used in simulations

Boundary	Boundary condition	Description
Inlet	Velocity = 0.1 m/s	Uniform flow profile
Outlet	Gage Pressure = 0 Pa	No pressure
Top Surface	Shear Stress = 0 Pa	Symmetry
Walls	Velocity = 0 m/s	No slip

Some assumptions were made in the simulations. It was assumed that the spherical produce did not rotate and move during washing but stayed in the fixed positions in the flume. Although this is an over simplification, it is a good starting point. In the simulations, gravity was ignored and the inlet flow velocity was assumed as uniform. There were no air bubbles created in the wash water and the effect of surface waves (in real life) on water surface was also ignored.

2.3.4. Changing the distance between two spherical produce

The first step of this segment was to examine how two spherical produce interact with each other in terms of their surface shear stress. Two edges were selected on the produce surface as shown in FIGURE 10. The shear stress value along the edges was then calculated by COMSOL® Multiphysics with its build-in functions. The horizontal

distance D between the upstream and downstream spheres was changed as shown in TABLE 3. It was expected that the upstream sphere should affect the shear stress experienced by the downstream sphere. However, the downstream sphere should not significantly affect the shear stress on the upstream sphere. One of the goals of this segment was to obtain the specific distance between which two spheres the shear stress experienced by one was not affected by the other. This information is useful in finding the maximum number of produce in one layer in a wash flume without sacrificing washing efficiency.

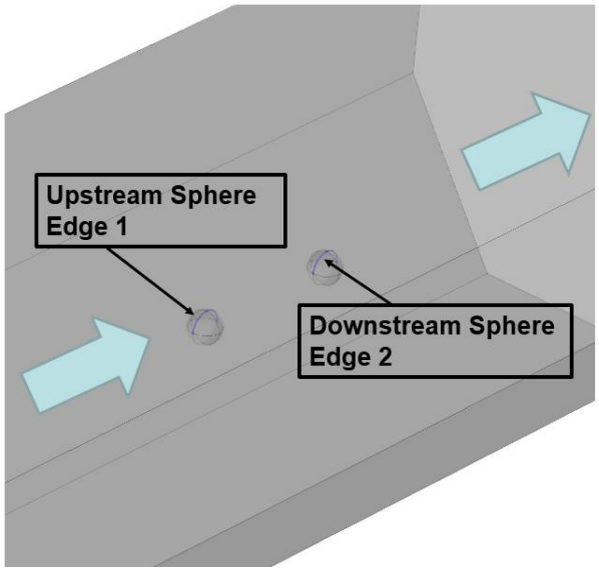


FIGURE 10 Upstream sphere and downstream sphere in the flume. The edge 1 and edge 2 were the top-half line of longitude on each sphere.

As shown in FIGURE 11, the spheres were touching each other in the beginning (simulation #1) and the distance between them was increased step wise, each step equaling the diameter of the spheres. In TABLE 3, the distance was normalized by dividing the actual distance by the sphere diameter.

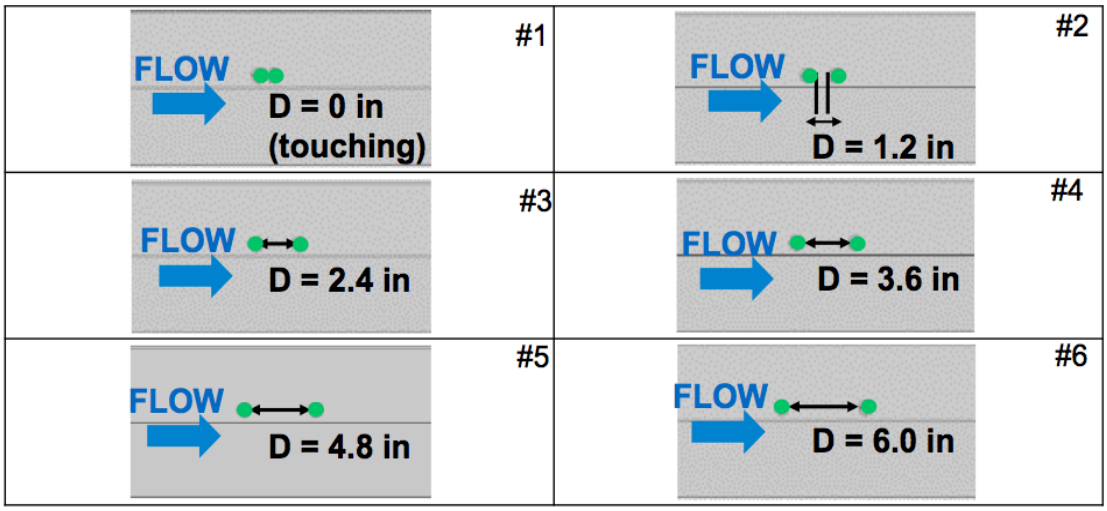


FIGURE 11 Side view 3D drawing with changing distance between upstream and downstream spheres.

TABLE 3 All the distance values used in simulations

Simulation#	1	2	3	4	5	6	7	8
Distance (in)	0	1.2	2.4	3.6	4.8	6	7.2	8.4
Distance / Diameter	0	1	2	3	4	5	6	7

2.4. Ordinary differential equations (ODEs)-based model for bacterial detachment and attachment in the flume washer system with given injected sanitizer concentration

The ODEs model that has equations (7), (8), and (9) was used to predict bacteria detachment and attachment in the flume washer. The concentration and values (X, B, and C) were uniform everywhere in the flume. There were no suspended bacteria in the wash water initially (when time equaled to zero). 6 logs CFU/cm^2 of bacteria were attached on the produce surface and, therefore, the concentration of bacteria in wash water (X) increased because bacteria started to detach from the produce surface at a rate that was governed by the detachment rate constant (k_{det}). Meanwhile, some of the bacteria detached from produce surface would re-attached onto the produce surface based on the attachment rate constant (K_{adh}). The chlorine sanitizer added in the wash water was used to inactivate the bacteria in wash water and thus reduced the total bacteria load in the washer system. As more and more produce was being added into the flume, the total organic matter increased and chlorine was depleted by the organic matter. Dilution of the bacterial concentration and sanitizer also happened during the washing process. The concentration of bacteria in wash water (X) and sanitizer concentration (C) decreased proportionally based on the dilution rate. The natural decay of chlorine also reduced the chlorine concentration (C). More importantly, chlorine mainly inactivates bacteria in wash water rather than on produce surface (Gil et al., 2009). In order words, only attachment and detachment rate constant affect the number of bacteria on the produce surface.

Based on the ordinary differential equations (ODEs)-based model, prediction of bacterial inactivation on a produce surface and in the wash water could be achieved. By changing those influential parameters in the ODEs such as detachment rate constant or chlorine concentration, this model could be used to optimize the processing conditions during produce washing in fresh produce industry.

2.4.1. Rationale for the ODEs

In order to apply the ODE model to a produce in the flume washer, the ODEs model was applied to a small cylindrical space, where X (wash water bacteria concentration), B (surface bacteria concentration), and C (sanitizer concentration) were uniform everywhere (refer to FIGURE 3). As for the mass balance, the number of bacteria introduced into this cylindrical space equalled to the number of bacteria attaching to the surface plus those being washed out. Based on the previous assumptions, bacteria concentration exiting the cylindrical space equalled to the average or uniform concentration X. The reason why only a small part of the surface area was selected was because bacteria detachment mainly happened on this small surface area based on the shear rate value, which will be discussed more specifically in the next section.

In the flume washer system, the situation of multiple spherical produce (more than 2 produce) in the flume was considered. In this case, total of 39 spheres were placed in one layer near the surface of the flume because this was the maximum number of spherical produce that this specific flume could hold while ensure their highest surface shear stress. The distance between each sphere was four times as their diameter, which was the minimum distance needed to ensure the maximum detachment constant and,

therefore, the highest washing efficiency. In FIGURE 12, the wash water was coming from the inlet on the left and exiting the flume from the outlet on the right. X, B, and C were only functions of time. The total effective surface area (A) was the sum of all the small areas on each sphere where detachment rate constant (k_{det}) was relatively higher than the other area on the surface. In other words, this layer of produce could be approximated as a flat surface where bacteria detachment and attachment happened. In this model, chlorine sanitizer was introduced at a fixed concentration from the inlet carried by the wash water.

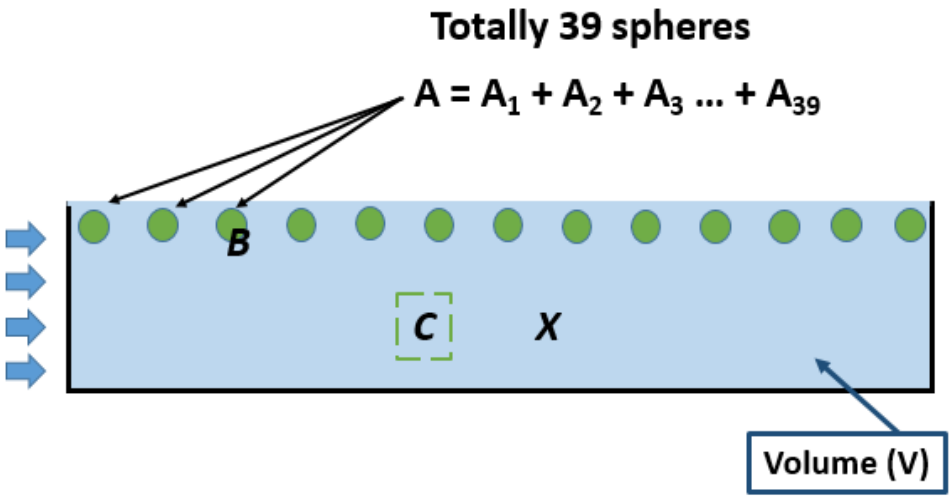


FIGURE 12 Ordinary Differential Equations (ODEs)-based model for the flume loaded with one layer of spherical produce.

2.4.2. Using the shear rate value to calculate detachment rate constant (k_{det})

The shear rate value and shear stress value along the selected line on surface was calculated. As shown in FIGURE 10 and FIGURE 13, COMSOL® Multiphysics calculated the shear rate value based on its build-in equations and given boundary conditions. The total arc length of the top-half longitude of the sphere was about 1.88 inches. According to FIGURE 13, surface shear rate started to increase when the arc length was 0.8 inches and reached the maximum value at about 1.25 inches. As shown in FIGURE 14, the shear rate values were then used to calculate detachment rate constant by equation (17) derived in the previous section.

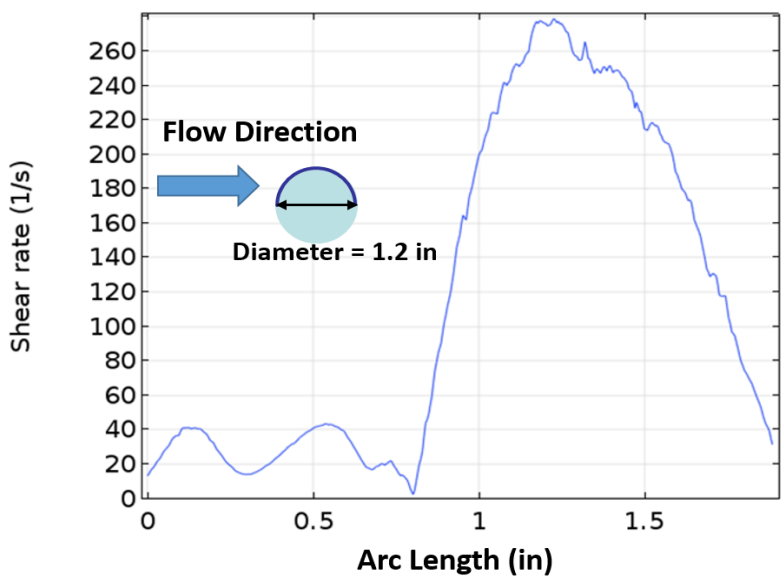


FIGURE 13 Shear rate values along the top-half of the longitude on sphere surface.

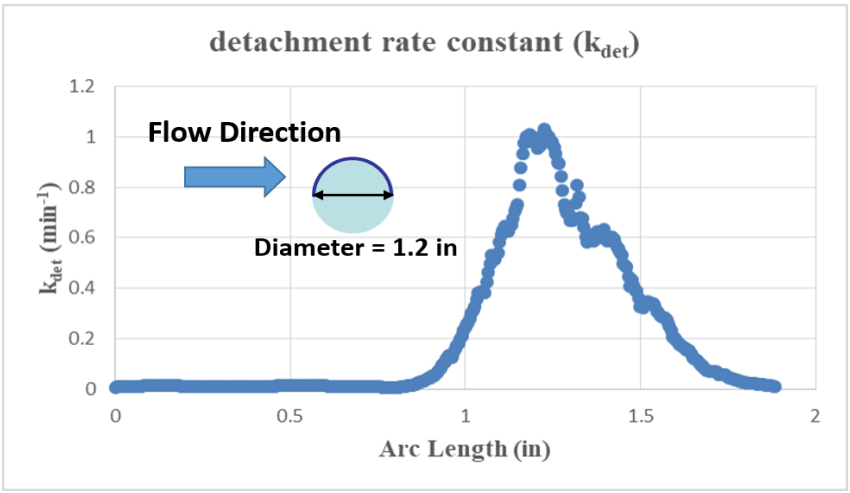


FIGURE 14 Detachment rate constant (k_{det}) along the top-half of the longitude on sphere surface.

According to FIGURE 14, detachment rate constant (k_{det}) value was close to zero when the flow hit the sphere on the "front". As distance along the arc length reached 0.8 inches, the detachment rate constant started to increase and reached the peak value. The average k_{det} was then calculated within certain arc range as shown in FIGURE 15. The reason to only select part of the arc length to calculate the average k_{det} was because detachment was mostly happening within this range.

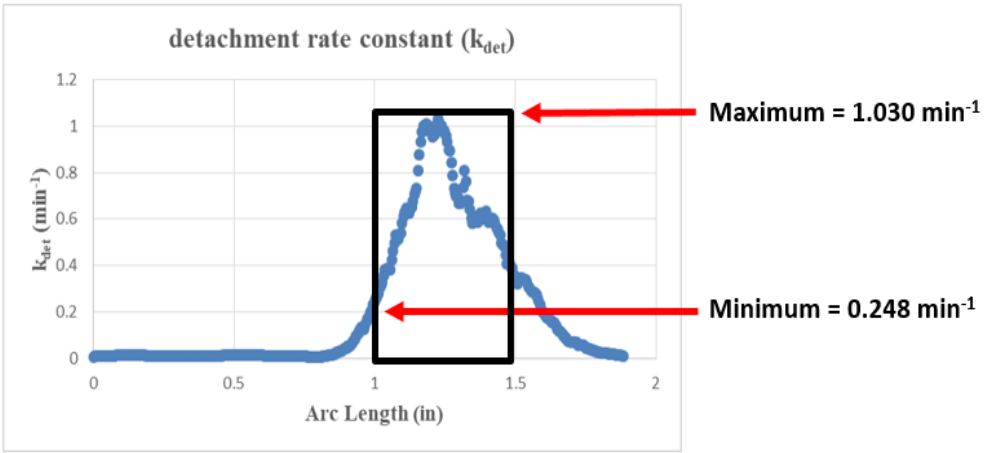


FIGURE 15 Arc where average detachment rate constant was calculated.

2.4.3. Values of parameters applied in the ODEs model

TABLE 4 Parameters used in the ODEs model

Parameters	Values	Descriptions	References
k_{det}	0.649 min^{-1}	Detachment rate constant	_ _
K_{adh}	0.01 cm min^{-1}	Adhesion rate constant	(Wang & Bryers, 1997)
A	52.13 cm^2	Total effective surface area	_ _
V	220.24 L	Flume volume	_ _
D	2.953 min^{-1}	Dilution rate	_ _
C_{in}	25 ppm	Inlet chlorine concentration	_ _
O	k_0t	Amount of organic matter	(Munther et al., 2015)
k_0	32.3 mg/(L min)	Increasing rate of organic matter	(Munther et al., 2015)
λ	1.7×10^{-3} min^{-1}	Natural decay rate of chlorine	(Munther et al., 2015)
α	0.75 L/(mg min)	Bacterial inactivation efficiency of chlorine	(Munther et al., 2015)
β	5.38×10^{-4} L/(mg min)	Chlorine depletion rate by organic matter	(Munther et al., 2015)

2.5. Chlorine distribution in the industrial-scale flume washer under different flow conditions

The same 3D geometry design of the flume washer was used to study the chlorine distribution under different flow velocity and injection ports location. The spheres representing produce was not included in the 3D design of the flume washer. A set of sanitizer injection ports were added on the bottom wall of the flume. There was no organic matter during the process and only dilution effect and natural decay of free chlorine were considered in the simulations. Considering the impact of the flow conditions on chlorine distribution, model to describe the change of chlorine concentration was developed based on related literatures (Munther et al., 2015; Wang & Bryers, 1997). The aim of this segment was to investigate how different flow settings and injection ports location affected the distribution of chlorine sanitizer during the process.

2.5.1. Geometry

Modified from the 3D flume geometry used in previous study, a new 3D geometry was created to simulate the mixing of chlorine sanitizer into the wash water in the flume washer. As shown in FIGURE 16, the flume had totally 6 injection ports on the bottom where free chlorine was injected into the flume. Shown in FIGURE 17, the distance between a pair of injection ports (side by side) were 4 inches and each pair of injection ports was 20 inches apart from the adjacent pair. The diameter of each injection port was 1.2 inches, which was designed to approximately resemble the industrial design. In the simulations, symmetry condition was used on the top surface representing the free surface where shear force equaled zero. Wash water with uniform chlorine concentration

at 15 ppm was the inlet condition. Chlorine was also injected from the bottom injection ports in the concentration of 50 ppm.

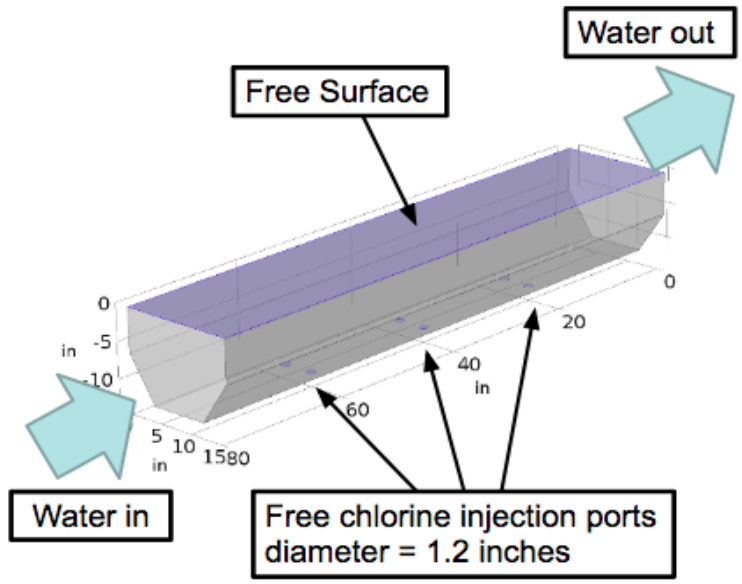


FIGURE 16 Geometry design of the flume with injection ports on the bottom

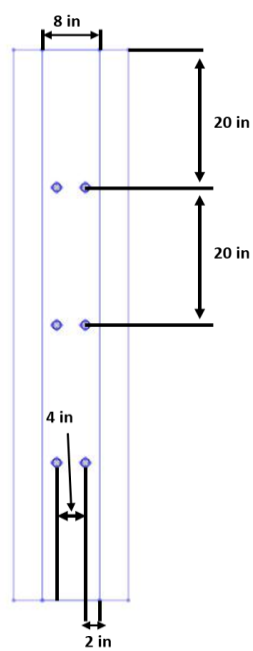


FIGURE 17 Bottom view of the flume washer with injection ports

2.5.2 Boundary condition and chlorine dynamics in turbulent flow system

Besides the effect of flow on chlorine distribution, a chlorine dynamics model was used to quantify the changing of chlorine concentration in the flume washer. As shown in equation (20), the term "$-\lambda C$" described the natural decay of free chlorine in accordance with its concentration inside the flume washer system (also see TABLE 4). Diffusivity of chlorine in water was taken as 1.25×10^{-9} m^2/s (Singh & Heldman, 2014). The complete 3D design is shown in FIGURE 18.

Total of four different flow conditions (flow velocity combinations) were simulated as shown in TABLE 5. The main flow velocity was the flow velocity of the wash water at inlet and the injection velocity was the flow velocity of the injected chlorine solution.

$$\frac{dC}{dt} = -\lambda C \qquad (20)$$

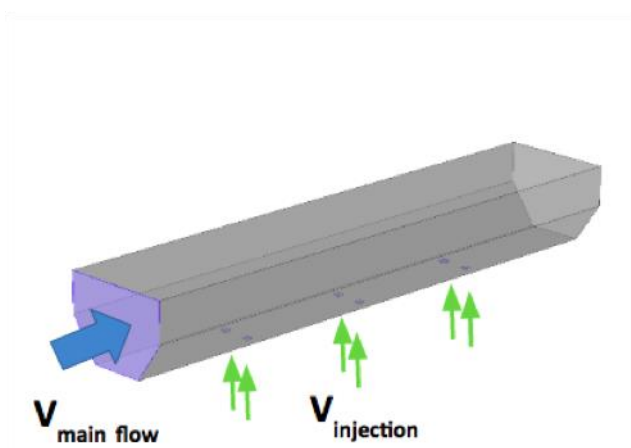


FIGURE 18 Injection of chlorine from the bottom

TABLE 5 Different flow conditions

$V_{injection}$ / $V_{main\ flow}$	0.3 m/s	0.2 m/s
0.2 m/s	Case #1	Case #3
0.1 m/s	Case #2	Case #4

The combination of 0.3 m/s injection velocity and 0.1 m/s main flow was gave the best mixing results based on results of the preliminary study. Therefore, the flow condition of which injection velocity equaled 0.3 m/s and main flow velocity equaled 0.1 m/s was selected to investigate the impact of injection ports locations on chlorine mixing in the flume washer. FIGURE 19 shows the 3D geometry of the flume washer with injection ports on both sides. There were total 6 chlorine injection ports and therefore 3 injection ports on each side. The injection ports on each side were 20 inches apart from adjacent ports. The distribution of chlorine at the outlet was then used to evaluate which design (bottom injection or sided injection) gave a better mixing of chlorine.

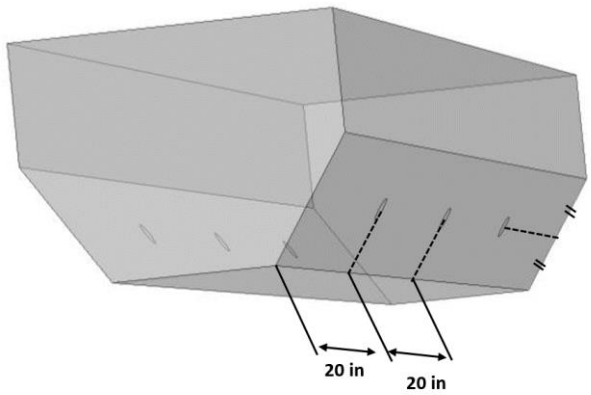


FIGURE 19 Flume with injection ports on the side panels

CHAPTER 3. RESULTS AND DISCUSSIONS

3.1. Numerical results of turbulent flow in the flume washer and the shear stress value on produce surface

Two spheres with 1.2 inch in diameter were placed in the flume washer representing spherical produce in the washing process. During the simulation, wash water was continuously flowing over the produce surface and therefore generated a certain amount of shear stress on the surface. The results showed how the shear stress on produce surface changed with the horizontal distance between two spheres in the turbulent flow.

3.1.1. Flow profile in the flume washer

According to FIGURE 20, the flow domain right after the spheres had flow separation bubble where the shear stress was low. From the side view 3D drawing in FIGURE 20, when the distance increased to certain value, the ‘tail’ of upstream spheres was separated from the downstream sphere, which means the upstream sphere was not blocking the downstream sphere and therefore the downstream sphere was able to fully expose to the flow to generate surface shear force.

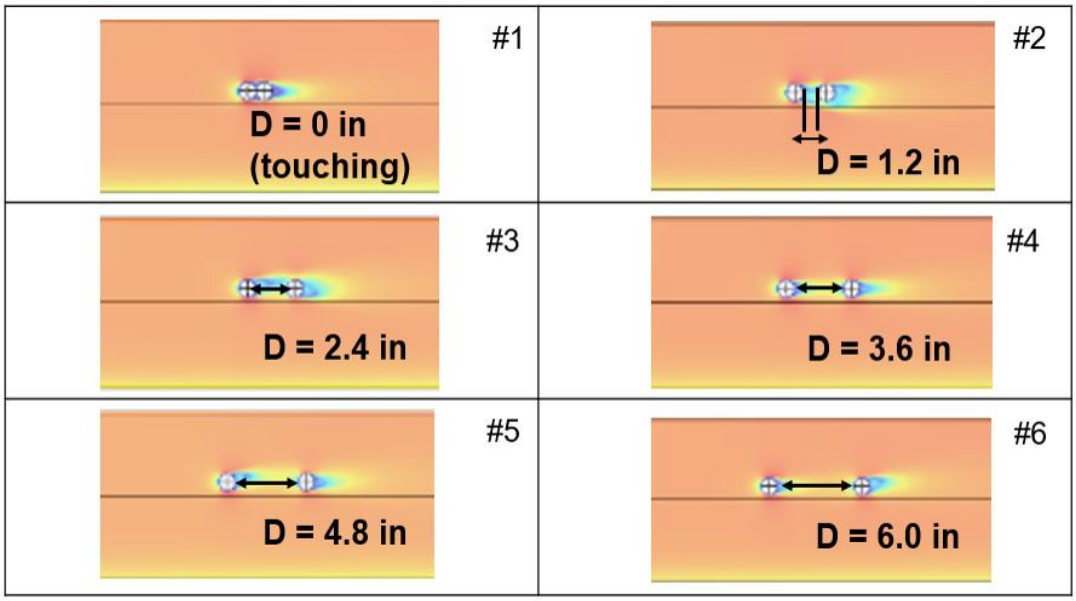


FIGURE 20 Side view velocity contours with changing distance between upstream and downstream spheres. Red or orange color represents high velocity and blue or green color represents low flow velocity. The flow was from the left to the right and flow velocity was 0.1 m/s.

3.1.2. The impact of distance between spherical produce on surface shear stress

As shown in FIGURE 8 and FIGURE 10, shear stress along selected arcs on each sphere surface was calculated during simulations. The arcs were defined as the longitude on the top-half surface of each sphere. Flow washed the sphere from the left to the right. More specifically, flow hit the sphere on its left. In other words, the flow first hit the spherical produce at the point that arc length equals 0 inch and flow past through top-half of the longitude of the sphere generating shear stress on sphere surface. FIGURE 21 shows the shear stress values along the edge of the upstream sphere when the distance between these two spheres was increased from 0 inch to 8.4 inches. The shear stress distribution followed a similar pattern as the distance increased, which indicated that the surface shear stress on the upstream sphere was least affected by the downstream sphere.

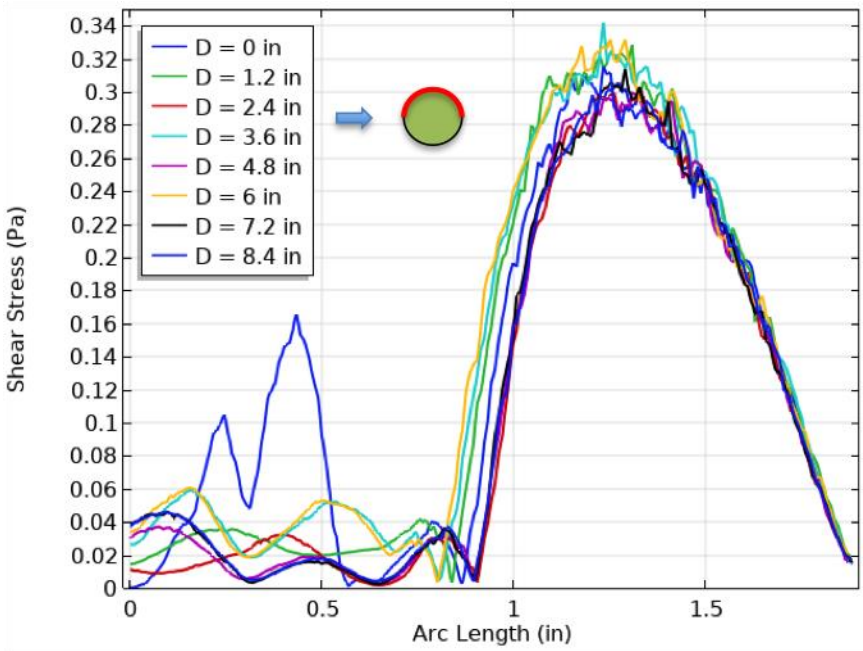


FIGURE 21 Shear stress values on the edge of upstream sphere

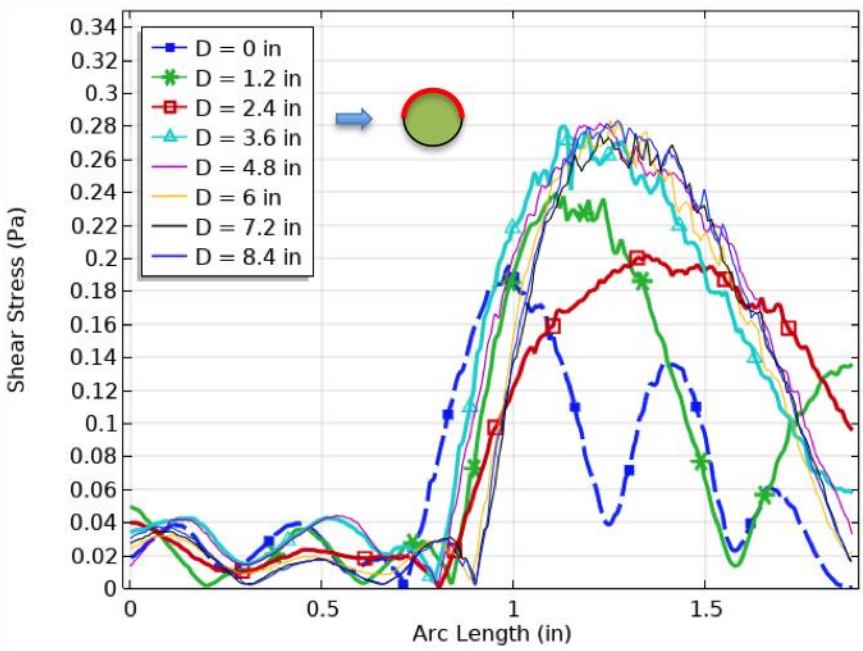


FIGURE 22 Shear stress values on the edge of downstream sphere

In FIGURE 22, the shear stress values were also calculated on the same arc of downstream sphere. As the distance between the downstream sphere and the upstream sphere increased, the surface shear stress on downstream sphere increased and approached the similar pattern as the upstream sphere. For all the scenarios, the maximum shear stress on the upstream sphere was about 300 mPa and the downstream was about 275 mPa. The shear stress values on the downstream sphere followed the same pattern as the upstream sphere when the distance was more than 4 times of the sphere diameter. To better visualize this change on shear stress, the shear stress values at a specific point where arc length equaled to 1.2 inches were selected and compared as a function of normalized (using diameter) distance between the two spheres as shown in FIGURE 23 and FIGURE 24. Based on the data, the shear stress values were unchanged after the distance reached 4 times of the sphere diameter. When the distance between two spheres reduced, the shear force on the downstream sphere was lower than the shear force on the upstream sphere. According to this, to maintain the highest shear force on each sphere, it is necessary to maintain the distance among spherical produce no less than four times as their diameter in this flume washer.

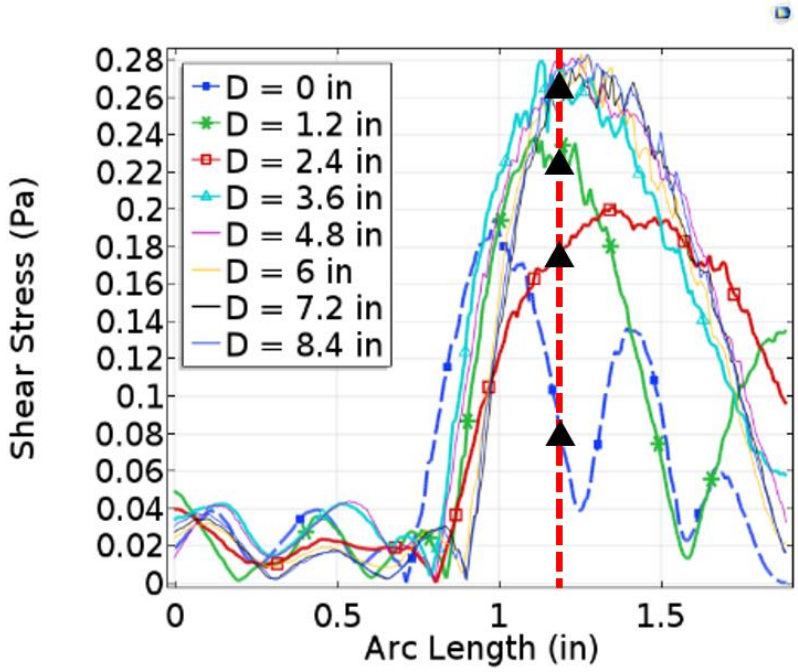


FIGURE 23 Selection of shear stress values at arc length equaled 1.2 inch on downstream sphere

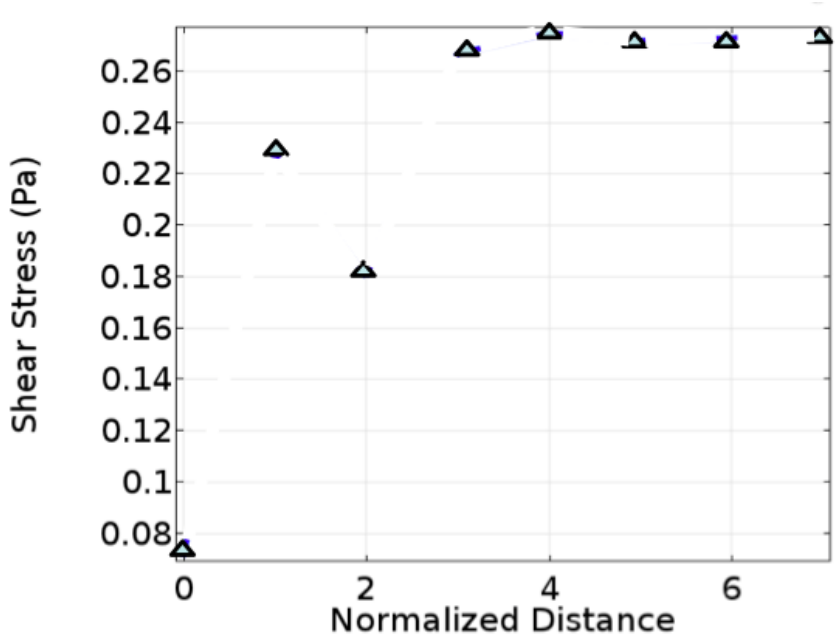


FIGURE 24 Shear stress values at arc length equaled 1.2 inch on downstream sphere

3.2. ODEs model results: prediction of bacterial inactivation

Based on the previous results that only investigated two spherical produce, multiple spherical produce were placed in the flume washer. To ensure maximum surface shear force, the distance between each of them was kept 4 times as their diameter. As shown in FIGURE 25, a layer that contained total of 39 spherical produce were placed in the flume washer. The number "39" was the maximal number of produce that could be fitted while ensuring the distance between each of them was 4 times their diameter.

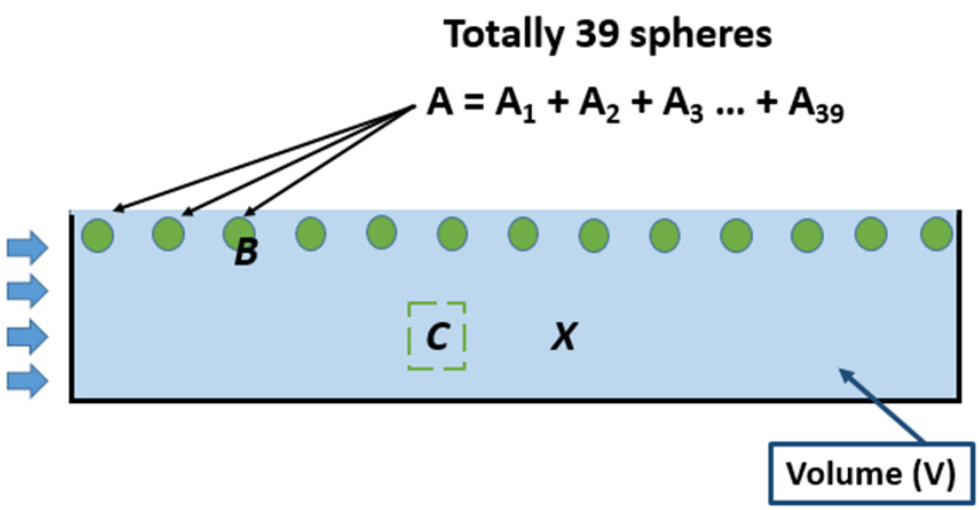


FIGURE 25 Repeating of FIGURE 12 Ordinary Differential Equations (ODEs)-based model for the flume loaded with one layer of spherical produce

FIGURE 26 shows the shear rate values calculated by using the downstream sphere. According to equation (5), shear rate was needed to calculate detachment rate constant (k_{det}). COMSOL® Multiphysics also has its build-in functions to calculate shear rate value on the sphere surface. FIGURE 27 shows the detachment rate constant values on the edge of each sphere. Based on this figure, only the area that had relatively high

detachment constant values was selected to study the microbial detachment and attachment. In FIGURE 28, only the part of the arc from 1 inch to 1.5 inches was used to calculate the average detachment rate constant. Within this arc length, the average detachment rate constant was calculated as 0.649 min^{-1}, the maximum was 1.030 min^{-1}, and the minimum was 0.248 min^{-1}. This average detachment rate constant was calculated by taking the average of all the data point within the selected arc length. The average detachment rate constant was then used in the ODEs model described by equations (7), (8), and (9).

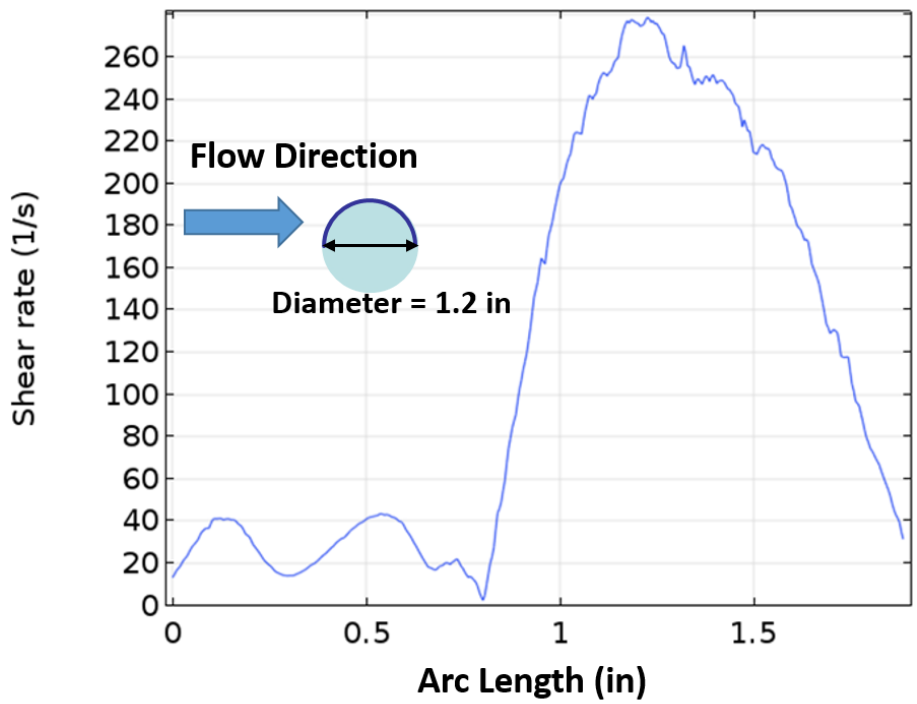


FIGURE 26 Shear rate values on the edge of downstream sphere

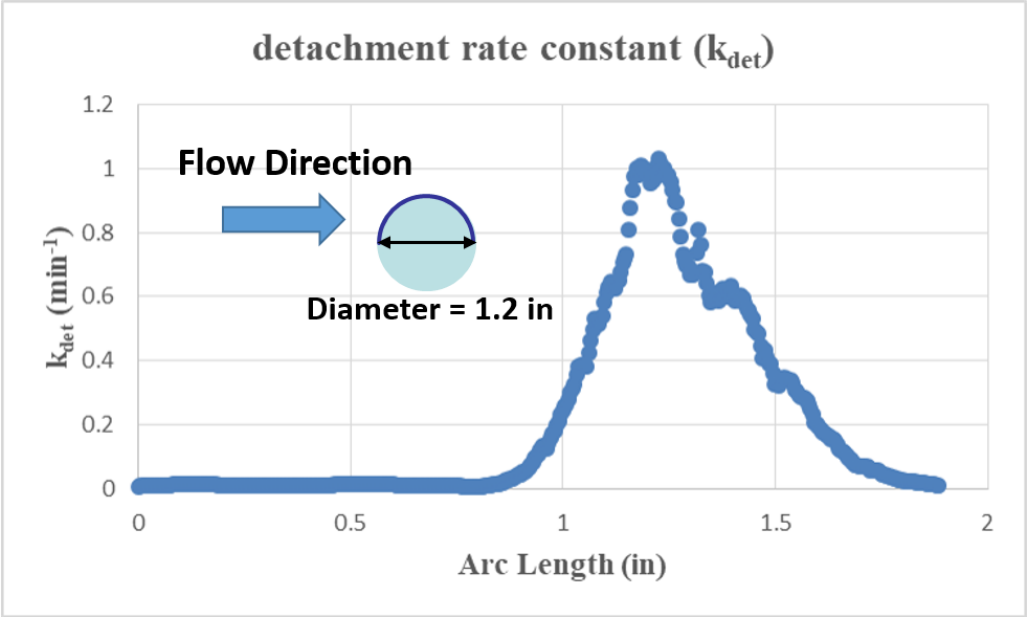


FIGURE 27 Detachment rate constant values on the edge of downstream sphere.

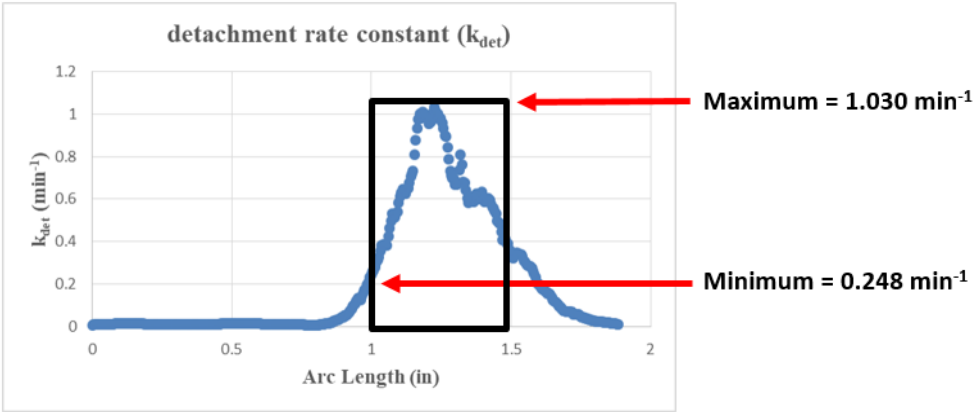


FIGURE 28 Calculation of average detachment rate constant within selected area

The ODEs model described in section 2.1 estimated the change of bacteria concentration in the wash water (X) from 0 minute to 2 minutes as shown in FIGURE 29 and FIGURE 30. The initial bacterial concentration in wash water was set as 0 and initial bacterial number per unit area on produce surface was 6 logs CFU/cm^2. The injected

chlorine concentration was 25 ppm. According to the figure, the number of bacteria was controlled lower than 3 logs CFU/ml from 0 minute to 2 minutes. In the parametric study, different curves represent the change of bacterial load under different values of detachment rate constant on produce surface. Besides the average k_{det}, the maximum k_{det} value and minimum k_{det} value were used in the ODEs. In addition, two more values of k_{det}, 10 times higher than the average k_{det} and 10 times lower than the average k_{det} were also used. FIGURE 29 indicates that higher k_{det} removed more bacteria from the produce surface into wash water where chlorine inactivated the bacteria cells. Therefore, bacteria on the produce surface would be detached into wash water more quickly due to the increased driven force as more bacteria were inactivated in wash water. As a result, most of the bacteria on produce surface would be removed from the surface and inactivate in the wash water. The ODEs model also estimated the number of bacteria on produce surface per unit area as shown in FIGURE 30, which indicated that the higher the k_{det} the lower the bacterial concentration on produce surface because most of the cells were detached by shear force wash water, which is not surprising.

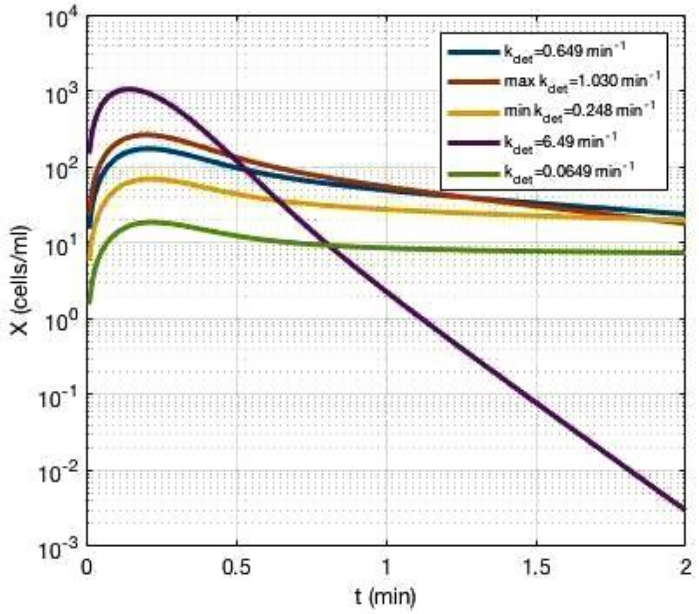


FIGURE 29 Number of bacteria in the wash water with different detachment rate constant on produce surface in the flume contained 39 spherical produce

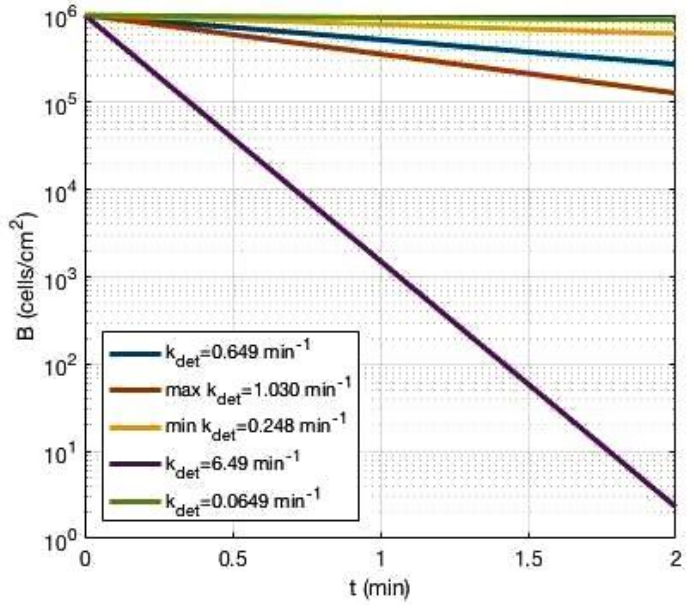


FIGURE 30 Number of bacteria on produce surface with different detachment rate constant on the surface in flume washer contained 39 spherical produce

During the washing process, the depletion rate by organic matter would be different if different sanitizers were used. FIGURE 31 shows an example of how the concentration of sanitizers were different within the 2 minutes time period. According to Munther et al. (2015), the depletion rate of chlorine by organic matter is 5.38×10^{-4} L/(mg min). When this value was increased by a factor of 10, the change in the sanitizer concentration should be different. FIGURE 31 shows the sanitizer concentration during the washing process.

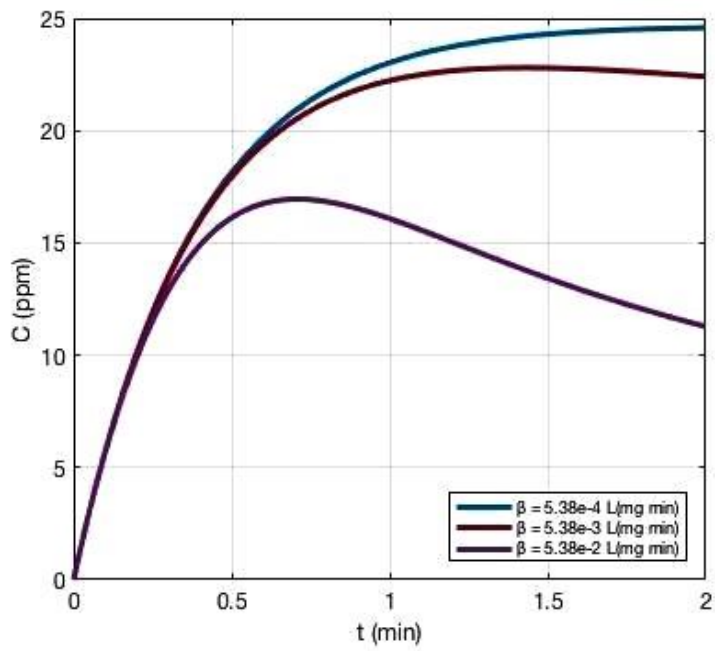


FIGURE 31 Chlorine sanitizer concentrations with different depletion rate by organic matter (β) in the flume washer contained 39 spherical produce

3.3 Numerical results of chlorine sanitizer distribution in the flume washer

3.3.1. Flow profile in the flume washer

The Reynolds numbers of both the injection port and flume main flow velocity were calculated based on formula and parameters from reliable sources (Schlichting & Gersten, 2017; Singh & Heldman, 2014). As shown in TABLE 6 and TABLE 7, all flow conditions could be considered as turbulent flow (Schlichting & Gersten, 2017; Singh & Heldman, 2014). According to the geometry design described in section 2.5.1, the chlorine was injected through the injection ports on the bottom of the flume and mixed with the main flow in the flume washer.

TABLE 6 Chlorine injection ports velocity (m/s) and Reynolds number

Velocity (v)	0.2 m/s	0.3 m/s
Reynolds number	6000 (turbulent)	9000 (turbulent)

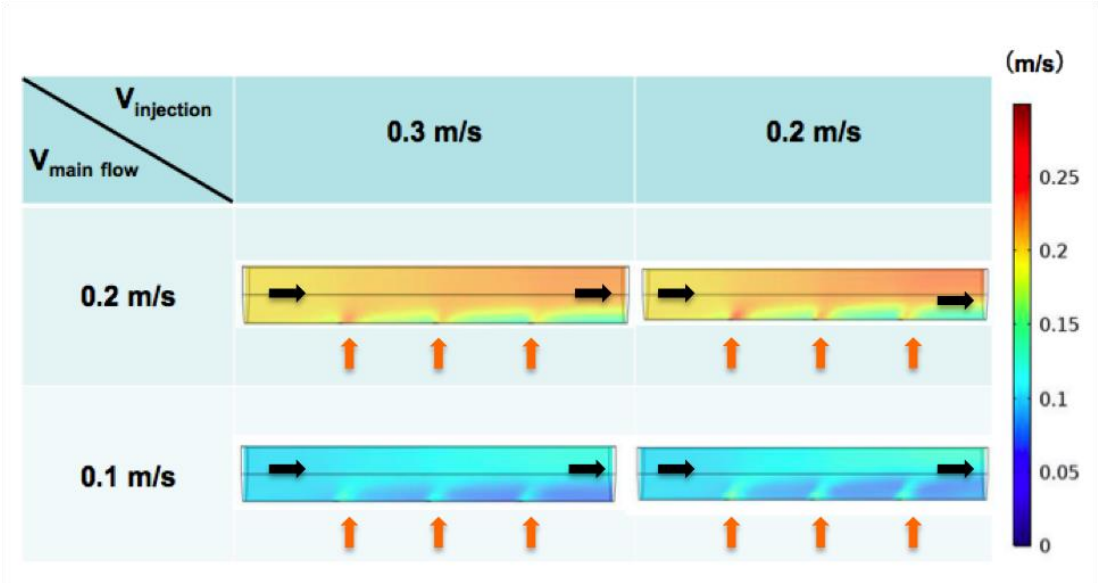
Note: Reynolds number = $\rho vD/\mu$, where ρ = 1000 kg/m^3, μ= 0.001 Pa s, D = 0.03 m (Singh & Heldman, 2014)

TABLE 7 Main flow velocity (m/s) and Reynolds number

Velocity (v)	0.1 m/s	0.2 m/s
Reynolds number	49700 (turbulent)	99400 (turbulent)

Note: Reynolds number = $\rho v d_h/\mu$, where ρ = 1000 kg/m^3, μ= 0.001 Pa s, $d_h = 4A/p$ = 0.497 m (Singh & Heldman, 2014)

TABLE 8 Total velocity Contours for the injection models



3.3.2. The impact of different flow conditions on the distribution of chlorine

In the study of chlorine distribution, the concentration of chlorine at the outlet was estimated by using COMSOL® Multiphysics. TABLE 8 shows the velocity contours for the injection models from a side view, in which chlorine was injected from the bottom and flow entered the flume on the left inlet and existed on the right outlet. FIGURE 32 shows the chlorine concentration contours at the outlet cross-sectional plane. Given the same injected 50-ppm chlorine from the bottom injection ports, lower main flow velocity gave higher average concentration than at high main flow velocity. The effect of injection velocity on chlorine distribution was much lower than the effect of main flow velocity. TABLE 9 shows the average concentration, maximum concentration, minimum concentration, and the coefficient of variation (COV) of chlorine at the outlet cross-sectional plane. According to the COV values of each case, lower main flow velocity also

provided better mixing of chlorine in the water. FIGURE 33 shows the effect of injection ports location on chlorine distribution. The flow conditions were same for both cases where main flow velocity was 0.1 m/s and injection velocity was 0.3 m/s. Injected chlorine was 50 ppm for both designs. According to FIGURE 33, side injection ports had higher average concentration at the outlet plane. Side injection also gave better mixing of chlorine sanitizer on the outlet.

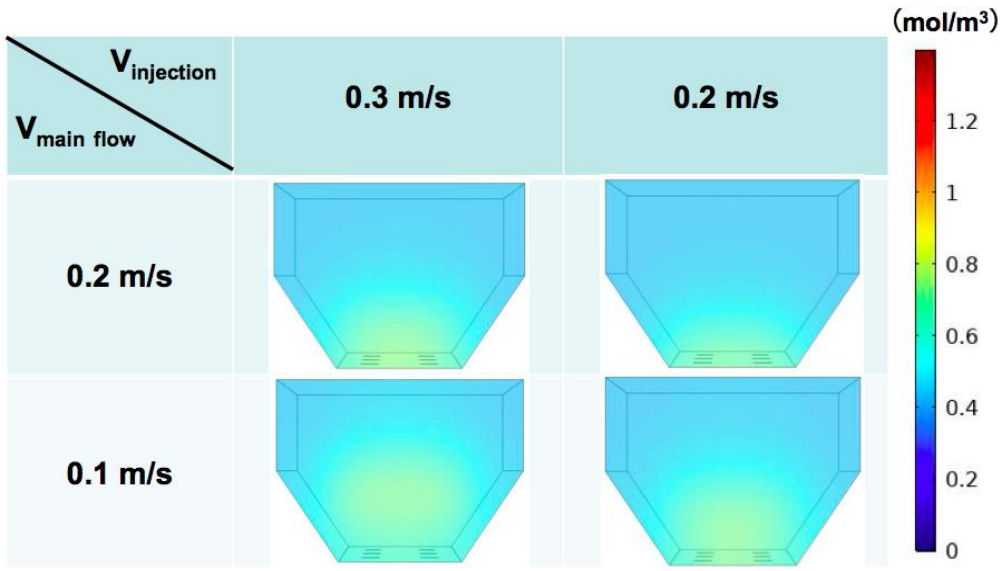


FIGURE 32 Concentration contours of chlorine distribution at the outlet plane of the flume under different flow conditions

TABLE 9 Average concentration of chlorine on the outlet plane of the flume under different flow conditions

$V_{main\ flow}$ \ $V_{injection}$	0.3 m/s	0.2 m/s
0.2 m/s	Average Conc. = 0.485 mol/m³ Max = 0.735 mol/m³ Min = 0.420 mol/m³ COV = 0.178	Average Conc. = 0.463 mol/m³ Max = 0.687 mol/m³ Min = 0.419 mol/m³ COV = 0.150
0.1 m/s	Average Conc. = 0.529 mol/m³ Max = 0.710 mol/m³ Min = 0.425 mol/m³ COV = 0.164	Average Conc. = 0.498 mol/m³ Max = 0.714 mol/m³ Min = 0.420 mol/m³ COV = 0.173

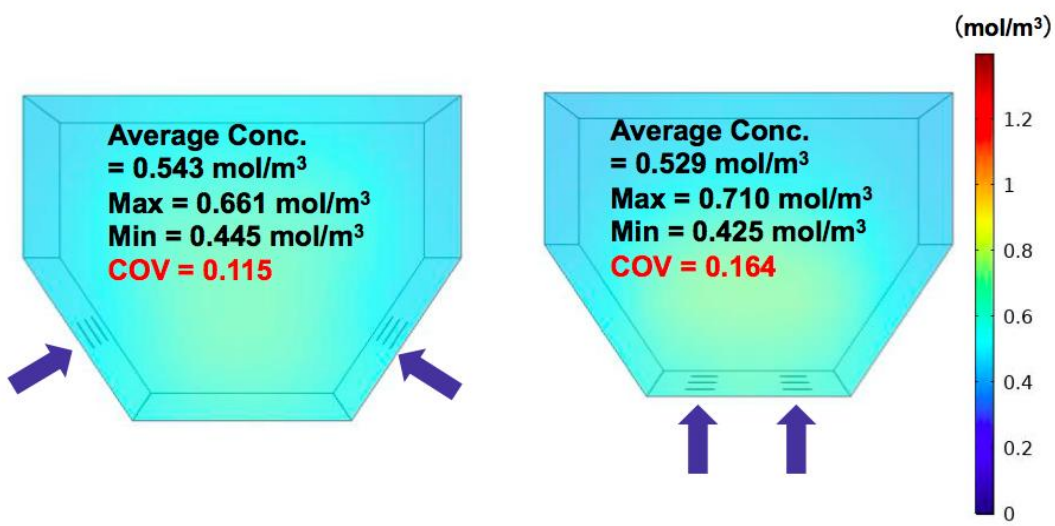


FIGURE 33 Comparison between sided injection and bottom injection in terms of chlorine sanitizer distribution

3.4. Closing Statements

With the addition of chlorine, the amount of bacteria in wash water reduced and was controlled under certain level. The numerical model demonstrated the combined effect of shear force and chlorine sanitizer during the produce washing process in an industrial-scale flume washer. The simulation also showed how bacteria were removed from the produce surface and being inactivated in the wash water during produce washing.

The simulations used dimensions and approximated values from the produce washing industry. However, due to the assumptions described in section 2.3, the validity of the numerical result has many points for improvement. The spherical produce was represented by spheres in fixed position in the flume, which may increase the surface shear stress because, as the sphere can be pushed by the flow, the relative flow velocity should be lower than the value used in this case. Rotation of the spheres should also reduce the shear stress on the surface. In the study of chlorine distribution, spherical produce was not present in the flume, which may have impacts on mixing of the chlorine. To improve the accuracy of these simulations, some assumptions should not be applied and therefore the spheres should be floating and rotating with flow inside the flume washer instead of in fixed positions. When simulating the chlorine distribution, organic matters should also be considered because organic matters causes a lot consumptions of chlorine during the washing process. However, the simulations in this study only considered the mixing of chlorine sanitizer and washing water. Last but not least, experiments should be conducted in actual produce washing processing line or pilot plant to validate the accuracy of these simulation results. Only the difference between

simulation results and experimental results is close enough, the simulations can be considered valid.

CHAPTER 4. CONCLUSIONS

The cross-contamination and inactivation of bacteria during the produce washing process were numerically simulated. The shear stress on produce surface was calculated according to the flow velocity. The surface shear stress was converted to the detachment rate constant (k_{det}). In the ODEs, attachment rate constant (K_{adh}) and detachment rate constant (k_{det}) were used to measure the cross-contamination of bacteria among each produce when wash water served as the media. Fixed amount of added chlorine was also included in the ODEs to inactivate the bacteria in wash water. The distribution of chlorine sanitizer inside the flume washer under different flow conditions were also studied. By comparing different injection velocity of the chlorine sanitizer and different injection port positions, an optimized flume washer design was developed. However, further validation experiments should be conducted to increase the accuracy of these simulations.

In a typical industrial flume washer, shear stress experienced by the downstream product will be lower than the upstream sphere unless the separation between the products is sufficient, i.e., four times as the diameter for a spherical produce. The maximum surface shear stress value was 275 mPa on the downstream produce. The microbial detachment rate constant on produce surface was correlated with inlet flow velocity of the flume washer. Based on their correlation, shear rate was converted to k_{det} (bacterial detachment constant). Increasing the inlet flow velocity, the bacterial detachment rate constant on produce surface increased. If the k_{det} value is higher, more bacteria will be detached from produce surface into wash water, where sanitizer inactivates the bacteria. Flow condition plays a significant role in distributing free

chlorine as a sanitizer in the flume washer. The sanitizer concentration can be numerically estimated based on the sanitizer depletion rate by organic matter. Overall, this model was used to numerically estimate bacteria load in washing water and on produce surface. The model was also used to estimate sanitizer efficiency in wash water over time. Injection flow velocity affects the free chlorine distribution in the flume washer. Injection ports location also affected the free chlorine distribution in the flume. Based on the results, lower injection (0.1 m/s) velocity gave more uniform distribution of the sanitizer than higher injection velocity (0.2 m/s). Side injection ports design is more efficient for sanitizer distribution than bottom injection design.

CHAPTER 5. FUTURE WORK

In the future, it is necessary to find the experimental and modeled relation between k_{det} to flow rate at different flow condition (laminar flow, turbulent flow, or mix) at high flow rate (> 0.3m/s). It is also very important to validate the mathematical results by doing on site experiments in the same or similar flume washer, which is bound to improve the accuracy of the model.

In terms of the methodology, it is necessary to replace the spheres with other geometry such as slices that represent lettuce leaves or rods that represent squashes. There are many varieties of vegetables and their unique geometry will have a great impact on the surface shear stress and mixing of the sanitizer in the flume washer system. Produce can flow with the flow and therefore the relative flow velocity and rotation of the produce should be considered in simulations. Therefore, fluid solid interaction between the wash water and produce should be simulated, which enhance this model to a more dynamic and realistic system.

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