Computational Fluid Dynamic (CFD) Simulation of

Droplet Impact Behavior on Rough Surface

by

Mohd Syaifullah Bin Ramli

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Universiti Teknologi PETRONAS

Bandar Seri Iskandar

31750 Tronoh

Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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A project dissertation submitted to the Chemical Engineering Programme Universiti Teknologi PETRONAS in partial fulfillment of the requirement for the BACHELOR OF ENGINEERING (Hons) (CHEMICAL ENGINEERING)

Approved by,

lah:

(AP DR. KU ZILATI KU SHAARI)

ASSOC. PROF. DR. IIU ZILAR IIU SHAAR Chemical Engineering Department Universiti Telunologi PETRONAS

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Junt Has

(MOHD SYAIFULLAH BIN RAMLI)

ABSTRACT

Coating of urea is a recent interest in agriculture which still needs a lot of research to increase the efficiency and effectiveness. Controlled-released urea (CRU) functions according to nitrogen demand pattern of the particular plant. Research on the droplet impact is performed to help in the prediction of the impingement behavior of these droplets for urea coating. However most of the studies and researches on this area currently focusing on a flat, smooth surface. Therefore this research is conducted to study the behavior of droplet impact on flat rough surface of different texture with various impact velocities. This project is intended to simulate the droplet impact behavior on rough surfaces using computational fluid dynamics (CFD) 2dimensional (2D) modeling based on the volume of fluid (VOF) approach by means of ANSYS FLUENT software. The liquid used as droplet is water and simulated at impact velocity of 3.0 m/s, 1.5 m/s and 0.5 m/s on roughness texture of 'triangle', 'square', 'curve' as well as smooth surface made of aluminum. Droplet spreading behavior of water droplet on surface of urea is successfully simulated using ANSYS FLUENT. In relation to coating coverage on the urea surface, the 'triangle' surface and 'curve' surface resembles closely to uneven surface of urea. To have 'square' surface is almost unlikely. Therefore it can be said that from the simulation, to have the best coating, low velocity of spray should be used to coat the urea which approximately around 0.5 m/s. Besides that, from the simulation result, the coating will be the best if the urea surface has the 'triangle' texture.

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CHAPTER 1

INTRODUCTION

1.0 INTRODUCTION

1.1 Project Background

Nitrogen (N) is an important element for plant growth and usually required in an ample quantities. In fact according to Hue (2009), after the invention of the process to produce artificial ammonia (NH_3), the usage of urea as fertilizer had increased over the years due to higher nitrogen contents than organic fertilizer which is used in the conventional farming system.

However, plants need different amounts of nitrogen at different stages of growth. The application of controlled-release urea (CRU) is favored over conventional urea. CRU improved nitrogen use efficiency. The gradual release of CRU provides nutrients at a rate which based on plants nutrients demand. Pipko (1990) states the urea fertilizer may be produced as chemically or physically.

Olson-Ruts et al. (2011) explain the methods of producing CRU discussed here use coatings (physically) to delay or extend the nutrient availability. Ku Shaari and Turton (2010) mentioned coating uniformity is essential particularly if the coating is for functional purposes, which here for the purpose of controlling the release of the urea fertilizer.

Tomaszewska & Jarosiewicz (2002) highlighted the advantages of CRU over the conventional type, such as lower rate of removal of the fertilizer from the soil by rain or irrigation water, sustained supply of minerals for a prolonged time, increased efficiency of the fertilizer, lower frequency of application in accordance with normal crop requirement, minimized potential negative effects associated with over dosage, and reduced toxicity.

The other advantage of CRU is the ability to somehow control the rate of plant-based food production against the demand. This is related to food security since the increasing of world population means higher food demand. This phenomenon eventually leads to the needs to enhanced current agricultural technique to meet the demand.

Olson-Ruts et al. (2011) reported environmental advantage of using CRU are less release of nitrate (NO₃) contamination and nitrous oxide (N₂O) which are greenhouse gases. N₂O or also known as 310 GWP CO₂ is one of the main sources of global warming. GWP CO₂ stands for Global Warming Potential relative to CO₂. In this particular case according to United States of Environmental Protection Agency, N₂O has 310 times potential more than CO₂ in 100 years. Less production of this gas could give quite significant effect to control global warming.

Besides that, CRU has the potential to reduce cost by applying the fertilizer only once. This reduction will minimize capital and operation cost, hence optimize the profit. Research on coating uniformity for CRU production will actually benefits the society.

Based on Turton (2008) the most important parameter related with coating method is the uniformity of the applied coating. There are two type of coating which are mass coating uniformity and uniformity related with coating morphology. The fact is the morphology of the coat is important in the quality control of coated products. Same amounts of coatings could be found on two coated particles however for some reason one of the particles does not has complete coverage, and then enteric protection would not be afforded. Imperfections in the coating layer could cause significant effect in the desired performance. There are several modeling techniques that can quantify important processing variables and are applicable to all coating process and one of them is computational fluid dynamics. In order to predict the droplet spreading behavior on the surface of urea particle, CFD will be used to simulate this phenomenon.

1.2 Problem Statement

Production of controlled-release urea (CRU) by coatings requires deeper research to increase the efficiency of the release according to nitrogen demand pattern of the plant. Olson-Ruts et al. (2011) stated that CRU-type fertilizer generally delay the release of nutrients, therefore the release timing is important. Moreover Ku Shaari and Turton (2010) mentioned the importance of coating uniformity and describe the fundamental principle of film coating is to provide a fine mist of coating solution that contains droplets, which will impinge onto the urea substrate.

In order to understand the coating coverage, research on the impact behavior of an individual droplet need to be performed to help in the prediction of the impingement behavior of these droplets (Ku Shaari & Turton, 2010).

For the past few decades, numerous researches and studies on the droplet spreading behaviour on surfaces have been conducted. These researches and studies comprise of theoretical studies, experimentation and as well as numerical methods. Nowadays most researches on this particular area are carried out using the aid of software, e.g. computational fluid dynamics (CFD) simulation method.

Therefore this research is conducted to study the behaviour of droplet impact on different texture of rough surfaces with various impact velocities to relate to the best urea coating method. This research will use the means of CFD simulation in order to observe the pattern and behaviour of droplet impact on the rough substrate.

1.3 Research Objective and Scope of Study

- To develop a Computational Fluid Dynamic (CFD) of 2 dimensional (2D) model based on the volume of fluid (VOF) approach by means of ANSYS FLUENT software.
- 2. To simulate the droplet impact behavior on different rough surfaces using computational fluid dynamic (CFD) of 2 dimensional (2D) model based on the volume of fluid (VOF) approach by means of ANSYS FLUENT software.
- To investigate the effect of droplet spreading behavior on different texture of rough surfaces with various impact velocity to relate to the best urea coating method.

1.4 Project Relevancy

Simulation of a droplet by using the ANSYS FLUENT software could gives better understanding of the droplet impact behaviour. However, the findings of the simulation still need to be validated through experiment.

1.5 Project Feasibility

Research by CFD simulation requires the fundamental knowledge of fluid dynamic, transport phenomena and differential equations. The combinations of these fields reflect the complexity of the research and thus will be strictly conducted step by step to ensure better understanding is attained. If required, consultation from expert will be requested.

It is assumed that the project is feasible within the scope and time frame with regard to software availability and the required expertise. The proposed Gantt chart with the milestone and expected due date is shown in the next section. The study and analysis will emphasize more on the behavior of droplet impact with various impact velocities on substrate of different roughness texture.

CHAPTER 2

LITERATURE REVIEW

2.0 LITERATURE REVIEW

The basic concept of controlled-release urea is that they release their nutrient contents at more gradual rates that permit maximum uptake and utilization of the nutrient while minimizing losses due to leaching, volatilization or excessive turf growth (Sartain, 2010). The important fact is the surfaces of urea particles are rough and uneven. This becomes a major challenge in investigating the droplet spreading behavior on the rough surfaces.

Single liquid droplets impact on a surface is a common phenomenon in many natural and industrial process such as pharmaceuticals, herbicides spraying, ink jet printing, spray cooling of hot surfaces, fuel injection of diesel engines, paint coatings, and in this research the focus is on coatings of urea fertilizer.

The prediction of a droplet impact behavior is rather complex due to a lot of influencing factors. The possible factors such as the diameter and the impact velocity of the droplet, properties of the liquid and the target surface and it may result in deposition on the surface, reatomisation into smaller secondary droplets, or in a complete rebound. Even though most of the studies and researches on droplet impact behaviour concentrate on the effect on a flat and smooth surface, the data and results can be used as initial predictions for the rough surface.

De Ruijter et al. (1999) describes there are two types of droplet spreading exist; hydrodynamic and molecular kinetic, which differs mostly in the consideration of the dominant dissipation channel. Hydrodynamic emphasizes the dissipation due to viscous flow generated in the core of the spreading droplet. From this approach, relation between contact angle $\theta(t)$ and the capillary number (*Ca*) is derived.

The second approach, which originates from the molecular theory, has been modified to describe the kinetics of wetting phenomena. This approach is in contrast to the hydrodynamic because it focuses on the processes happening in the environment of contact line which barricade from the attachment of fluid particles to a solid.

According to experimental observation by Marengo et al. (2002), the impact of the droplet can be categorized in four (4) phases which are the first stage represents (1) the kinematic phase, followed by a (2) spreading phase where all the other parameters begin to play a role in the impact evolution. The spreading phase is followed by a (3) relaxation phase, which may have different outcomes, depending mainly on the magnitude of the receding contact angle. In a final phase, the lamella decelerates strongly and attains some constant diameter, (4) equilibrium phase) or, for highly wettable surfaces, continues slowly to wet the surface.



Figure 1: Schematic representation of the spread factor with time. The different lines correspond to an arbitrary choice of possible spreading histories, depending on the parameters of the impact. (Morengo et al., 2002)

Garbero et al. (2002) state most of the works concerning spreading have been addressed towards the two extreme conditions: impact at high Weber (We) and Reynolds (Re) numbers, where spreading is driven by impact velocity, or slow spreading of highly viscous liquids, at very low Reynolds numbers, driven by capillary effect at the contact line.



Figure 2: Dimensionless Number

The dynamics of spreading are mainly characterized by We and Ohnesorge (Oh) numbers and in the final part of the spread, by the contact angle. The Weber number takes into account inertia and elastic force due to surface tension. At high We inertia predominates over surface tension ones and the lamella quickly expands till reaching a large diameter and a thin thickness, before starting the retraction phase. At small We it is surface tension that predominates and thus a shorter spreading phase occurs, followed by an accelerated recoiling.

The Oh number scales viscous dissipation with elastic forces, that is, the two forces that contrast spreading. Viscosity is mainly responsible for the resistance at high values of the Oh, while surface tension effect is predominant at low Oh. Changing the liquid properties, the drop diameter and the impact velocity, four regions can be distinguished as a function of We and Oh. At small We and Oh the impact occurs at relatively small velocities and surface forces govern the spread phenomenon. As a consequence, the contact angle between liquid and surface becomes important. Here the dissipation due to viscous forces can be neglected since the velocity is low.

At high values of We and small Oh the spread mainly depends on the impact dynamic pressure. Viscous dissipation can be neglected in the first phase of the spread, where impact velocity and drop size are the controlling parameters, while it become significant when the lamella approaches it maximum size. At high values of Oh and small We the velocities are low, the spread is controlled by the surface forces and the high viscosity quickly damps all the velocities. In the last region, high Weand high Oh, the drop impacts the surface with high velocity and the liquid has a high viscosity and a small surface tension. The spread is controlled by the inertia and the dissipation by the viscous force is remarkable.

Analysis by Morengo et al. (2011) find out the impact of drops on solid surfaces implies the knowledge of the effects of wettability on the dynamic of the spreading. During the initial stages of the drop impact the effect of wettability is very low, since the flow in the spreading lamella is mainly governed by inertia. The surface wettability becomes important only when the lamella has a very low velocity, since only then does the adhesion forces start to play a role.

Also wettability, in particular the dynamic contact angle dependence on contact line velocity, governs the drop receding motion which in some cases (non-wettable smooth surfaces and relatively low We) can lead to drop rebound.

The surface wettability, also according to Morengo et al. (2011) has an important role on the behavior of the liquid lamella rupture for high velocity drop impacts. The film rupture occurs for impact velocities above a given threshold Re, which depends on the receding contact angle. Interestingly enough there is a minimum value of this threshold Re for intermediate contact angles, while both low and very high contact angles tend to stabilize the film behavior (correspond to higher threshold Re).

Effect of wettability is characterized by a static (or equilibrium) contact angle. For most of the actual surfaces the value of the equilibrium contact angle is not unique but lies in a range between the static receding and static advancing contact angles. The liquid starts to spread if the contact angle exceeds the static advancing contact angle. Correspondingly, the process of dewetting is initiated at the angles below the static advancing contact angle (Marengo et al., 2011).

Morengo et al. (2011) also mentioned that the substrate wettability is usually not accounted for in the development of the models for splashing threshold, since its influence on drop spreading at high impact velocities is negligibly small. Nevertheless, wettability plays a significant role in the splash produced by a solid spherical particle impacting into a water pool. Particle hydrophobicity enhances splash and air entrapment. We cannot therefore exclude completely the substrate wettability as a possible influencing parameter for splash also during drop impact onto a dry substrate.

A droplet impacting onto a smooth surface normally forms a liquid disk, called lamella, which expands very quickly and reaches a maximum diameter, d_m . Subsequently the lamella tends to shrink due to surface tension and to reach its final shape. The maximum extent to which a droplet spreads is a crucial parameter not only in those processes, described above, in which the whole impact phenomenon is reduce to the spreading phase, but also in other applications where splash, rebound or reatomisation may happen.

The prediction of the final area covered by a droplet is in strictly related to its d_m , since the lamella at this point has its maximum elastic energy and zero velocity. A change of the shape of the lamella can lead to large velocity variations during the recoiling phase and, as a result, modify strongly the outcome of the impingement.

Maximum spread, according to Garbero et al. (2002) can be predicted using the application of energy conservation approach which the total energy owned by the drop before impact is equal to that of the lamella at its maximum diameter minus the energy dissipated by friction.

The maximum diameter, d_m is one of the parameters of major interest in coating process because it related closely with the prediction of the final aspect of the target surface which in this case porous surface. In a coating process, variation of liquid viscosity and surface tension of the liquid, in conjunction with its shear thinning/thickening behavior will affect the outcome of the droplets impact.



Figure 3: Electron microscopy of uncoated urea particles

2.1 Roughness of the Surface

The actual surface of urea substrate, based on Ku Shaari and Turton (2010), could be rough and porous. A porous surface could provide less coating coverage and rough surface could cause splashing.

In 1996, Range and Feuillebois studied the influence of surface roughness on liquid droplet impact. They used different type of rough plates; plates with random profile of roughness, plates with regular grooves and plates with equal cavities. They observed that the splashing behavior is more dramatic on the plates with regular grooves. Results of their experiment are shown in Figure 4.

Experiment results	Description
	Water drop impact on commercial aluminum plate. Roughness, $R_{a} = 0.4365$ µm; Impact velocity = 3.54 m/s
•	Water drop impact on Plexiglass with equal cavities. Roughness, $R_d = 12.3383$ μ m; Impact velocity = 2.16 m/s
2	Water drop impact on Plexiglass with rectangular grooves. Roughness, $R_a =$ 20.170 μ m; Impact velocity = 2.16 m/s
	Water drop impact on Plexiglass with triangular grooves. Roughness, $R_a =$ 23.053 μ m; Impact velocity = 2.16 m/s

Figure 4: Experimental results of different surface roughness on liquid droplet impact (Range and Feillebois, 1998).

Katagiri et al. (2005) studied the spreading behavior of an impacting drop on a structured rough surface. The rough surfaces are specially prepared with a regular pattern of surface asperities (as in Figure 5). The major physical parameters that influence the drop impact process are the size and velocity of the drop prior to the impact, the liquid properties of the drop, and the surface characteristics of the solid surface. The drop parameters are grouped in terms of non-dimensional numbers such as Weber number (We); the ratio of inertial to surface tension forces, and the Ohnesorge number (Oh); the ratio of viscosity to surface tension forces.



Figure 5: (a) Texture pattern of the substrate and (b) magnified view of the asperities (Katagiri et al., 2005).

From the experiments that were conducted, they concluded that on structured rough textured substrates, an impacting liquid drop spreads simultaneously both inside the grooves and above the texture pattern of the substrate. For the impact of high We drops, the liquid flowing inside the grooves of the textured substrates jet spreading dominates the spreading process. The spreading diameter measured for the liquid volume flowing above the texture pattern of the substrate is smaller than that on the smooth surface, mainly attributable to the decrease in the liquid kinetic energy available above the texture pattern.

2.2 Impact Velocity of the Droplet

Oukach et al. (2010) reported that impact velocity has significant effect on droplet spreading where it produces significant changes in the shape of the splat. Increasing the impact velocity consequently increases spreading time as well as the spreading diameter of the droplet, and therefore the spreading factor.



Figure 6: Spread factor evolution during the flattening for different impact velocities (Oukach et al., 2010).

At high impact velocity, it should be noted that phenomenon of splashing occurs as droplets are forced out from the rim of the lamella at the end of flattening; in which kinetic energy exceeds the surface tension force.

It was also observed that in his report, droplet readily recoils and retracts for the surfaces with high contact angle and lower velocity. When system is less wetted, the splashing occurs early; i.e., splashing occurs at 50 ms for contact angle of 120° and 60ms when contact angle is 10° .

2.3 Computational Fluid Dynamic (CFD) Simulation Method

Much work has been done to predict the droplet spreading behavior on rough surface via experiment as well as simulation. However, CFD approaches to model the droplet spreading behavior on different surface roughness particularly that of a urea particle is still noticeably missing.

Ku Shaari (2007) performed studies on the effect of surface roughness on the spreading behavior of a droplet on flat surfaces with different roughness at ambient temperature. A static angle of 65° is used together with velocity of 0.5 m/s on 'fine', 'smooth', 'rough' and 'very rough' surface. The results showed that droplet spreading diameter decreases as surface become rougher. This is because the friction on a smooth surface which has less energy dissipation assists in retaining the kinetic energy of the droplet, causing the droplet to continue spreading. The surface area with a 'very rough' surface generally has more surface area compared to that of smooth surface, Figure 7 shows the spreading factor of droplets simulated on different surface roughness.



Figure 7: The spreading factor of the droplets simulated on different surface roughness (Ku Shaari, 2007).

Oukach et. al (2010) has investigated deformation behavior of a liquid droplet impacting a solid surface by using COMSOL Multiphysics for the simulation. Water droplet with a diameter of 3 mm is used and a contact angle 120° is chosen with velocity of 1.18 m/s in 2D and 3D simulations. Before impact, droplet has a spherical shape and upon impingement, it starts to spread where a thin film forms at the solid surface. As the diameter increases, the thickness of the droplet decreases as can be seen in Figure 6. At t = 4.7 ms, the droplet reaches its maximum spread and a raised rim is formed at the margin of the lamella due to increase of the mass by the surface tension forces which thwart the spread and decelerate the motion of the splat at the margin.



Figure 8: Impact and flattening of a 3.0mm water droplet with a velocity $v_o = 1.18$ m/s, (a) 2D simulation, (b) 3D simulation and (c) experimental result carried out by R. Rioboo (Oukach et al., 2010).

2.4 Volume of Fluid (VOF)

Volume of Fluid (VOF) method is commonly used in CFD simulation and was introduced by Hirt and Nichols. According to Balachandran (2009) VOF can be applied for flows comprises of two or more fluids. It is a volume-tracking technique in which the interface is tracked in a fixed grid using a scalar function called the volume fraction, F.

Hence, the interface is not tracked explicitly but computed using the values of F computed inside the domain. For a flow of two fluids, F = 1 indicates region having one fluid and F = 0 indicates that the region is completely filled by the other fluid. Void regions, where none of the two fluids are presence, is not allowed. Also the two fluids are assumed to share the same momentum equation, implying that the VOF method is not suitable for cases where the difference in the velocity between the two fluids is significant. It is included as Eulerian methods which are characterized by a mesh that is either stationary or is moving in a certain prescribed manner to accommodate the evolving shape of the interface.

2.4.1 Surface Tension

Surface tension arises as a result of attractive forces between molecules in a fluid. The addition of surface tension to the VOF calculation results in a source term in the momentum equation. The importance of surface tension effects is determined based on the value of two dimensionless quantities; the Reynolds number (Re) and the capillary number (Ca) or between Re and the Weber number (We). For Re << 1, the quantity of interest is Ca:

$$Ca = \frac{\mu U}{\sigma} \tag{1}$$

and Re >> 1, the quantity of interest is the We:

$$We = \frac{\rho L U^2}{\sigma} \tag{2}$$

where U is the free-stream velocity.

Surface tension effects can be neglected if Ca >> 1 or We >> 1.

2.4.2 Wall Adhesion

The contact angle that the fluid is assumed to make with the wall is used to adjust the surface normal in cells near the wall. This dynamic boundary condition results in the adjustment of the curvature of the surface near the wall.

If θ_w is the contact angle at the wall, then the surface normal at the live cell next to the wall is:

$$\hat{n} = \hat{n}_w \cos\theta_w + \hat{t}_w \sin\theta_w \tag{3}$$

Where \hat{n}_w and \hat{t}_w are the unit vectors normal and tangential to the wall. The combination of this contact angle with the normally calculated surface normal one cell away from the wall determine the local curvature of the surface, and this curvature is used to adjust the body force term in the surface tension calculation. Figure 7 illustrates the measurement of contact angle.



Figure 9: Schematic diagram of the contact angle between phases (FLUENT Inc. ©, 2003).

An approach consist of solving the Navier-Stoke equations for the air and the liquid phase by means of a Computational Fluid Dynamics (CFD) and predicting in detail the transient flow field. By using models like the Volume of Fluid (VOF) the size of the liquid lamella is computed and the interface between liquid and air is traced.

CHAPTER 3

METHODOLOGY

3.0 METHODOLOGY

3.1 Modeling – ANSYS FLUENT

The fundamental basis of almost all Computational Fluid Dynamics (CFD) problems is the Navier-Stokes equations. The motion of fluids is describe by these equations. A virtual system can be built and then real world physics and chemistry can be applied to the model. The software will generate data and images, which represent the performance of the design. Computers are used to perform the millions of calculations required to simulate the interactions of liquids and with surfaces defined by boundary conditions.

ANSYS FLUENT software will be optimized to model the spreading behavior of a droplet. There are three major processes in the development of the model. (1) Domain identification and mesh development, which is the most important part. It is necessary to have equal nodes on every sides of the model. Selection of optimum meshes size and time step for the simulation will determine the accuracy of the modeling.

Next step, (2) is to set up the solver and properties. Examples of properties that need to be set up are the chemical and physical properties of the droplet and the boundaries conditions.

Finally, (3) the final steps are the model initialization and solution monitoring or in other words run the simulation. A little work is required in this step since most of the solver and properties has been prepared.

3.2 Assumptions of the Model

- 1. The ambient air is stagnant.
- 2. The liquid droplet is spherical at the time of impact.
- 3. The liquid is incompressible with constant surface tension and viscosity.
- 4. Newtonian and laminar fluid.
- 5. No-slip boundary condition along the solid surface with no penetration.
- 6. The boundary condition does not include evaporation.

3.3 Research Methodology

3.3.1 Grid Size Study

Before determine the optimum mesh size and time step size for running the simulation, grid size study needs to be done. The purpose of the grid size study is not only for simulation to run smoothly but it also saves time as well as cost while doing the project. Table 1 and Table 2 summarize the grid size and time step size values which were used to enhance the simulation.

Table 1: Grid Size Study

Mesh	Size (mm)
	0.200
	0.150
	0.100
	0.075
	0.050

Table 2: Time Step Size

Time Step Size (s)
$1 \ge 10^{-08}$
1 x 10 ⁻⁰⁷
1 x 10 ⁻⁰⁶
1 x 10 ⁻⁰⁵
1 x 10 ⁻⁰⁴

3.3.2 Mesh Development

A domain has to be developed to the flow system before the dynamics of flow can be simulated. In this project as mentioned before, ANYSY DesignModeler is used to generate a geometry and grid of the flow domain used in the model. The dimensions of the geometry are 2.2 mm \times 40 mm illustrated in Figure 10. The grid size or more properly known as mesh was set to 0.05 mm x 0.05 mm. This selection of grid size will be discuss further in the next section.



Figure 10: Dimension of the geometry, 2.2 mm × 40 mm (x-axis and y-axis respectively).

Similar domain are created with different texture of rough surface are structured along the y-axis to simulate the uneven surface of the area. These are then used to study the effect of the rough surface towards the spreading behavior of the droplets. 3 models of rough surface were generated and the parameters are shown in Figure 11. Figure 12 summarize the images of the meshed flow domain for the three different texture of rough surfaces; 'square', 'triangle', and 'curve'.



Figure 11: Different roughness texture, 'square', 'triangle', and 'curve' respectively.



Figure 12: Meshed flow domain of 'square', 'triangle', and 'curve' respectively.

3.3.3 Model Setup

In the model, two phases are specified, Phase 1 and Phase 2. Phase 1 is defined as air while phase 2 is defined as water-liquid. Phase 1 has to be incompressible gas to improve the solution solubility.

The model in this work requires a time-dependant solution, an explicit scheme from the VOF formulation was applied to the volume fraction values:

$$\alpha 1_{qq}^{i+1} + \rho_q^{i+1} + \sum_f (\rho_q J_f^i \alpha_{q,f}^i) = \left[\sum_{p=1}^i (\dot{m}_{pq} - \dot{m}_{qp}) + S_{aq} \right] V$$
(4)

Where i + 1 is the new time step, i is the previous time step. α_{qf} is the face value of the q^{th} volume fraction, V is the volume of cell and J_f is the volume flux through the face, based on normal velocity.

From this scheme, the time step size can be determined. To ensure that the fluid uses up enough time in a cell, selecting the time step size is important to assist in convergence. The time step size for the volume fraction depends on the maximum Courant number, *Co* which is defined by:

$$Co = \frac{\Delta t}{\Delta x/v} \tag{5}$$

Where Δt is the time step size, Δx is the size of a cell in the x-direction and v is the fluid velocity or the impact velocity. The *Co* is set to 0.25 by default. For the volume fraction, the resulting time step is the time taken by the fluid to empty the cell.

3.3.4 Parameters

To study the spreading behavior of water droplet on the surfaces, several parameters needed to be taken into considerations which are as the Table 3 below:

Table 3: Physical properties of water droplet

Density	1000 kg/m ³
Viscosity	0.001 Pa.s at 20°C
Surface Tension	72.8 dynes/cm at 20°C

In this project as well, the impact of different velocity of the droplet towards its spreading behavior would be taken into consideration on the spreading of the droplet. Table 4 shows the different velocity which is used to study the effect on the spreading behavior as well as the contact angle. Contact angle (Figure 13) is defined as the angle between the tangent to the liquid interface and the tangent to the solid surface at the contact line between three phases. The contact angle is kept constant through out the simulation.

Table 4: Impact velocities of water droplets

Impact Velocity (m/s)	Contact angle
0.5	90°
1.5	90°
3.0	90°



Figure 13: Contact angle

3.3.5 Solution Initialization and Iteration

The volume fraction for phase 2, which is water-liquid droplet, is assigned to a value of 1. The particular impact velocity in negative y direction is specified. Once the material has been selected and set, water-liquid is patched into the flow domain that was created earlier. Figure 14 shows the initial form of the flow domain after the spherical region has been patched into the domain of smooth surface using ANSYS FLUENT.



Figure 14: Initial condition of the flow domain after phase 2 (water-liquid is patched into the system)

In summary, to simulate the initial impact behavior of liquid-water, a volume of fluid (VOF) multiphase model was developed. A 2D model was used in this work due to its simplicity.

The simulations are run using grid size of 0.05 mm \times 0.05 mm with a time step of 1×10^{-06} second. The wall adhesion term in the boundary condition panel was activated to enable the use of contact angle. The surface tension and contact angle are set be constant at 73.5 dynes/cm and 90° respectively. The model is run in a 2-phase setting, with air as the main phase and water-liquid as the secondary phase. Three different types of roughness texture; 'triangle', 'square' and 'curve' were also developed and using the same parameters as the smooth surface, the spreading behavior of the droplets is also simulated.

The droplet has a spherical shape of 2.0 mm diameter. Such diameter is chosen since it is in the range of diameter which is widely used to study this phenomenon; between 1 mm to 3 mm. The solid surface used is Aluminum. The model is used to show the effect of different roughness texture and impact velocity on the spreading behavior of the droplet.

3.4 Gantt Chart

Table 5: Gantt Chart for FYP I

3																
	Details Week	1 2	3	4	'n	9	7		~	9	10	=	12		13	14
-	Selection of FYP Topic															
7	Meetings with supervisor															
ę	Preliminary research work and literature review															
4	Seminars															
ŝ	Prepares Extended Proposal							reak						Vabilo		
9	Extended Proposal submission (03/07/2013)							Sem B						оН вүв		
5	Prepares for Proposal Defence							biM						A insH		
00	Proposal Defence (10/07/2013)															
6	Prepares Interim Report															
6	Submission of Interim Draft Report															
10	10 Interim Report submission															•

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Table 6: Gantt Chart for FYP II

No.	Details	Week 1	7	~	+	-10	9	r-		~~~	6	10	=	12	13	1
-	Submission of Progress Report															
7	Meetings with supervisor															
ъ	Simulate droplet spreading behavior on a flat surface.															
4	Seminars															
S	Study the effect of visocity of droplet spreading on a flat surface.								K							
9	Simulate droplet spreading behavior on rough surfaces.								n Breal							
7	Study the effect of roughness texture and impact velocity on droplet spreading behaviour								rə2-bil							
00	Pre-SEDEX								N				•			
6	Submission of Dissertation (Soft Bound)									•					•	
10	Submission of Technical Paper														•	
П	Oral Presentation															•
12	Submission of Dissertation (Hard Bound)															•

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3.5 Key Milestone

For the objectives to be accomplished there are several milestones to be completed.

No.	Milestones	Duration
1.	Mesh development using ANSYS 14.5	September 2013
2.	Simulate droplet spreading behavior on a flat smooth surface.	September 2013
3.	Grid size study for optimum mesh size on the surface of urea.	October 2013
4.	Simulate droplet spreading behavior on a flat smooth surface.	October 2013
5.	Study the effect of droplet spreading on a flat smooth surface.	October 2013
6.	Simulate droplet spreading behavior on different roughness texture.	November 2013
7.	Study the effect of droplet spreading on different roughness texture and different impact velocity.	November 2013
8.	Submission of Dissertation	December 2013

Table 7: Key Milestone

CHAPTER 4

RESULT AND DISCUSSION

4.0 RESULT AND DISCUSSION

Yoon (2006) describes droplet impacting a surface may cause three scenarios to occur which are 'spreading', 'splashing' and 'rebounding' (as shown in Figure 15). These scenarios depend on the properties of droplet as well as the surface. The fluid properties that affect droplet impact behavior include droplet size, impact velocity, surface tension, viscosity and temperature. For the surface, the roughness and surface energy are known to have some influence on the behavior of the droplet impact.



Figure 15: Three major scenarios of droplet impact behavior (Yoon, 2006)

In the case of simulation of water droplet, it is observed that 'spreading' occurs at low impact velocity and when the impact velocity is increasing; 'splashing' starts to appear. In this study, velocity of less than 1.5 m/s is considered as low impact velocity and more than 3.0 m/s is considered as high impact velocity. For water droplet, 'rebounding' is not observed due to weak surface tension, low viscosity as well the type of the solid surface which not favors for the water droplet to rebound. According to Richard & Quèrè (2000), water droplet can rebound on highly hydrophobic surface. On this surface, the contact angle is nearly 180°, therefore the kinetic energy of the impinging drop can be transferred to surface energy without spreading and can fully bounce.

According to Marengo et al. (2002), the impact of the droplet can be categorized in four phases (Figure 16) which are the first stage represents (1) the kinematic phase, followed by (2) spreading phase where all the other parameters begin to play a role in the impact evolution. The spreading phase is followed by (3) relaxation phase, which may have different outcomes, depending mainly on the magnitude of the receding contact angle. In a final phase, the lamella decelerates strongly and attains some constant diameter, (4) equilibrium phase) or, for highly wettable surfaces, continues slowly to wet the surface.



Figure 16: Phases of droplet impact

The effect of roughness texture on droplet spreading is evaluated by spreading factor. The spreading factor is illustrated in Figure 17 where it is defined as the ratio of the droplet in the surface at time t, to the initial droplet diameter at time t_o .



Figure 17: Definition of spreading factor

Spreading Factor =
$$\frac{D_t}{D_o}$$
 (6)

Besides the effect of roughness texture, the velocity impact is also investigated further throughout the project. The study of the initial spreading of a droplet provides important information on the maximum spreading diameter, which also gives the coating coverage resulting from the droplet impact which in this case refers to coating coverage of urea surface. Grid size study is important to determine the optimum grid as well as the time step size for the simulation. The relationship between the grid size and time step size is given by:

$$\Delta t = \frac{\Delta x}{V_f} \tag{7}$$

Where Δt is the time step size, Δx is the grid size measured in the x-direction, and V_f is the fluid velocity in the cell. The magnitude of the Δt should be estimated to result a small Δx than the grid size. Based on the maximum Courant number allowed near the free surface, Δt is then defined automatically.

For the time step size, it is found out that time step size of, 1×10^{-07} and 1×10^{-08} provide similar results. Moreover, time step size of less than 1×10^{-06} , is too short and the movement of droplet cannot be analyzed. Thus, time step size of 1×10^{-06} is chosen since it is time saving and provides optimum simulation data. The optimum grid size used for this simulation is 0.05 mm \times 0.05 mm. This can be observed in Figure 17, that reducing the grid size will push the data to a threshold value which in this case the value of less than 0.05 mm will produce the same result with longer simulation time.



Figure 18: Water liquid fraction versus time with various grid sizes to determine the optimal grid.

After patching the spherical droplet shape onto the domain, it can be observed that in bigger mesh (grid size), the edge of the spherical shape is uneven while on the grid size of 0.05 mm, the edge is smooth and even.

4.2 Simulation Results



4.2.1 Effect of Droplet Impact Velocity on Spreading Factor





Spreading Factor vs Time on 'Triangle' Surface'

Figure 20: Graph of spreading factor vs time on 'Triangle' Surface.

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Figure 21: Graph of spreading factor vs time on 'square' surface.



Figure 22: Graph of spreading factor vs time on 'curve' surface.

Figure 18 to Figure 21 shows the graphs of spreading factor against time on smooth surface, 'triangle' surface, 'square' surface and 'curve' surface at impact velocity of 0.5 m/s, 1.5 m/s and 3.0 m/s.

For the spreading factor, d_o is defined as the diameter of the water droplet before the impact which is 2 mm and d_i is the spreading diameter at time t. As can be observed from the graphs, impact velocity of 3.0 m/s has the highest spreading factor and followed by 1.5 m/s and 0.5 m/s respectively. Therefore increasing impact velocity will increase the spreading factor.

It is also observed that at impact velocity of 3.0 m/s and 1.5 m/s which are simulated in the duration of 6.0 ms on all surfaces, the spreading factor can only be determined at certain period of time due to splashing and droplet break up. Thus, the observation for spreading factor only limited for a certain period of time for each texture.

Generally, all graphs initially increase exponentially and reach its limit at certain spreading factor value. It can be said that increasing impact velocity will increase the spreading factor.

4.2.2 Effect of Roughness Texture on Spreading Factor



Figure 23: Graph of spreading factor vs Time at impact velocity of 3.0 m/s.

Figure 23 shows the results of the simulation of water droplet spreading factor on smooth surface as well as rough surface of different texture; 'triangle', 'square' and 'curve' at impact velocity of 3.0 m/s.

At this high impact velocity, the focus is on the time taken for the water droplet to splash and break apart. Based on the graph in Figure 23, splashing occur earliest on 'square' surface, followed by 'triangle', smooth and 'curve' surface. Splashing occurs due to kinetic energy exceeds the surface tension as well as the substrate texture which will be discuss in the latter section.



Figure 24: Graph of Spreading Factor vs Time at impact velocity of 1.5 m/s.

Figure 24 shows the results of the simulation of water droplet spreading at impact velocity of 1.5 m/s. At this impact velocity, the spreading factor is also difficult to be determined due to splashing and droplet break up. However during the period of 6.0 ms, the droplet on smooth and 'curve' surface manage to spread without break up or splash / little splash.

At this impact velocity, splashing occur earliest also on 'square' surface and followed by 'triangle' surface. According to the Figure 23 and Figure 24, splashing on 'square' surface occurs approximately at the same time which is at 1.9 ms. Meanwhile for 'triangle' surface, it occurs at different time for both figures which are at 2.9 ms and 4.9 ms.

Spreading factor is only comparable between smooth surface and 'curve' surface. Obviously the smooth surface has higher spreading factor compares to 'curve' surface. This observation is predicted since according to Ku Shaari (2007), rougher surface provides more surface are and promotes more friction, therefore slowing down the spreading.



Figure 25: Graph of Spreading Factor vs Time at impact velocity of 0.5 m/s.

Figure 25 show the results of the simulation of water droplet spreading factor at impact velocity of 0.5 m/s. As compared to graphs from Figure 23 and Figure 24, the observation period is longer in Figure 25 which is 10.0 ms. These are due to lower impact velocity requires longer time to spread in which more number of time steps is applied.

However it is unexpected that water droplet on smooth surface and 'square' surface will experience break up at 6.0 ms and 10.0 ms, respectively (refer to Figure 34 and 35). For this reason and in order to compare the spreading factor at this velocity as well as to other impact velocities, duration of observation is limited to 6.0 ms.

Initially at impact velocity of 0.5 m/s, the smooth surface has the highest spreading factor which are followed by 'square', 'triangle' and 'curve' surface'. However after 3.9 ms, the spreading on 'square' surface is reducing and the order of the spreading factor changes to 'smooth', 'triangle', square' and 'curve' until the end of the period.

4.2.2 Effect of Roughness Texture on Droplet Impact Behavior



Figure 26: The simulation images of the spreading dynamic of a 2 mm water droplet on smooth surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 3 m/s.

Oukach et al. (2010) describes:

The droplet has a spherical shape before impact, and immediately after impingement, it starts to spread. A lamella (a thin film) forms on the solid surface, develops and expands horizontally with a radial velocity higher than that before the impact. Thus its diameter increases very rapidly while its thickness decreases.

Figure 26 shows the results of the simulation of water droplet on smooth surface at impact velocity of 3.0 m/s. It is discussed before at this velocity, the spreading factor is difficult to determine due to splashing and droplet break up.

Based on Figure 26, the droplet starts to splash as early at 0.9 ms which can be observed at the both ends and the splashing happens symmetrically. Gradually the thickness of the lamella decreases due to high kinetic energy and reaches the lowest thickness at 3.9 ms and at 4.9 ms, and break ups. High impact velocity induced the droplet to spread faster and has a bigger diameter.



Figure 27: The simulation images of the spreading dynamic of a 2 mm water droplet on 'triangle' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 3.0 m/s.

Figure 27 shows the results of the simulation on 'triangle' surface at impact velocity of 3.0 m/s. Based on Figure 27, the droplet starts to splash at 1.9 ms which can be observed at the both ends. However, the splashing behavior is different compared to smooth surface and it is asymmetrical.

On smooth surface, the splash occurs along the surface as small particle meanwhile on 'triangle' surface, the splash is more due to sharp edge of the triangular-shape substrate, while the slanted surface of the 'triangle' absorb some of the momentum and allows only little spreading.

It also reaches the lowest thickness at 3.9 ms and break ups at 4.9 ms. However, as mentioned before the spreading is much lower compared to smooth surface.

Figure 28 shows the results of the simulation on 'square' surface at impact velocity of 3.0 m/s. Based on Figure 28, the droplet starts to splash as early as 0.9 ms which is at the same time as smooth surface. The splash occurs along the surface as small particle which can be seen at both ends. It reaches the lowest thickness at 4.9 ms and at 6.0 ms it splash greatly.



Figure 28: The simulation images of the spreading dynamic of a 2 mm water droplet on 'square' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 3.0 m/s.

This behavior is because of the sharp edge of the square-shape and the particle collision of the entrapped water inside it. The effect of contact angle in this situation is insignificant since the effect of impact velocity obviously dominates the behavior.



Figure 29: The simulation images of the spreading dynamic of a 2 mm water droplet on 'curve' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 3.0 m/s.

Figure 29 shows the results of the simulation on 'curve' surface at impact velocity of 3.0 m/s. Based on Figure 29, the droplet spreads steadily and the thickness of the droplet decreases until it starts to splash at 4.9 ms.

As compared to previous textures; 'triangle' and 'square', 'curve' surface allows the water to spreads smoothly. The 'curve' texture absorbs the momentum whereas the sharp edge of 'triangle' and 'curve' promotes splashing. Aside of the surface area, the volume of 'curve' surface which can contains water is bigger compares to 'triangle' and 'square' surface makes the droplet spreads less.



Figure 30: The simulation images of the spreading dynamic of a 2 mm water droplet on smooth surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 1.5 m/s

Figure 30 shows the results of the simulation on smooth surface at impact velocity of 1.5 m/s. At this velocity, splashing is absent on smooth surface. This can clearly be compared with Figure 26. The droplet spreads steadily and almost symmetrically. The thickness of the lamella decreases by time and reaches the lowest thickness at 4.9 ms and starts to break up at 6.0 ms. However due to lower kinetic energy, the spreading is less as compares to impact velocity of 3.0 m/s.



Figure 31: The simulation images of the spreading dynamic of a 2 mm water droplet on 'triangle' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 1.5 m/s.

Figure 31 shows the results of the simulation on 'triangle' surface and based on the figure, the droplet did not splash. The effect of sharp edge of the triangular-shape substrate is less significant at impact velocity of 1.5 m/s. The thickness of the droplet decreases by time and reaches the lowest thickness at 3.9 ms and starts to break up at 4.9 ms. The spreading is also less as compares to impact velocity of 3.0 m/s.



Figure 32: The simulation images of the spreading dynamic of a 2 mm water droplet on 'square' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9, 6.0 ms respectively at impact velocity of 1.5 m/s.

Figure 32 shows the results of the simulation on 'square' surface. Among all the roughness texture at impact velocity of 1.5 m/s, only on this surface splashing occurs. This shows that the square-shape texture has significant effect on splashing of at least until 1.5 m/s.

The droplet starts to splash at 2.9 ms which is later than impact velocity of 3.0 m/s which is at 0.9 ms. The splash occurs along the surface. It reaches the lowest thickness at 4.9 ms and at 6.0 ms it just starts to break up. At this velocity, the particle water entrapped inside the 'square' collides weakly and contains the space. Contact angle probably has some significant effect on the splashing behavior.



Figure 33: The simulation images of the spreading dynamic of a 2 mm water droplet on 'curve' texture rough surface at t=0.0, 0.9, 1.9, 2.9, 3.9, 4.9 and 6.0 ms respectively at impact velocity of 1.5 m/s.

Figure 33 shows the results of the simulation on 'curve' surface and it is observed that the droplet spreads steadily along with the decreasing thickness. As discussed previously, 'curve' surface allows the water to spreads smoothly with no splash and no droplet break up.

Figure 34 shows the results of the simulation on smooth surface (left) at impact velocity of 0.5 m/s. At this velocity, longer observation time is used since the kinetic energy is too low and took longer time to spread. The duration is up to 10.0 ms, which previously 6.0 ms for impact velocity of 1.5 and 3.0 m/s.

Splash is completely absent at this velocity and particularly on smooth surface. The droplet spreads steadily and symmetrically. The thickness of the lamella decreases slowly by time and reaches the lowest thickness at 8.9 ms and break up at 10.0 ms. Spreading is much less as compares to impact velocity of 3.0 m/s as well as 1.5 m/s.



Figure 34: The simulation images of the spreading dynamic of a 2 mm water droplet on smooth surface (left) and 'triangle' surface (right) at t= 0.0, 0.9, 1.9, 2.9, 3.9, 4.9, 5.9, 6.9, 7.9, 8.9, and 10.0 ms respectively at impact velocity of 0.5 m/s.



Figure 35: The simulation images of the spreading dynamic of a 2 mm water droplet on 'square' surface (left) and 'curve' surface (right) at t= 0.0, 0.9, 1.9, 2.9, 3.9, 4.9, 5.9, 6.9, 7.9, 8.9, and 10.0 ms respectively at impact velocity of 0.5 m/s.

Figure 34 also shows the results of the simulation on 'triangle' surface (right) at impact velocity of 0.5 m/s. Splash is also absent on this particular surface. The droplet spreads steadily and almost symmetrically with the presence of trapped air inside the droplet.

The thickness of the lamella decreases slowly by time and reaches the lowest thickness at 7.9 ms and later experiencing a little recoil. Spreading is less as compares to smooth surface at the same impact velocity.

Figure 35 shows the results of the simulation on 'square' surface (left) at impact velocity of 0.5 m/s. No splash is observed. The droplet spreads symmetrically and the thickness of the lamella decreases slowly by time and reaches the lowest thickness at 6.9 ms and break up at 7.9 ms.

Figure 35 also shows the results of the simulation on 'curve' surface (right) at impact velocity of 0.5 m/s. Splash is absent and the droplet spreads and the thickness reduced until 6.9 ms before recoils. The recoils occurred is very obvious compared to recoiling on 'triangle surface'.

From the observation of the simulation results as well as the graphical analysis, it can be concluded that at high impact velocity, the spreading factor is difficult to be determined due to splashing and droplet break up. Meanwhile at low impact velocity, splashing is completely absent.

Also at low impact velocity, the smooth surface has the highest spreading factor and followed by 'triangle', 'square' and 'curve' surface. It also must be noted that the roughness textures do not show consistent order of spreading factor between the different impact velocities.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.0 CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Prior to the simulation, grid size study is done to optimize running time for the simulation. From the results, it shows that time step of 1×10^{-06} is the best time step size and the grid size of 0.05mm x 0.05 mm is the most favorable grid size to run the simulation.

A VOF multiphase model of 2.0 mm droplet is developed to predict spreading behavior of a droplet on rough surface. Different roughness texture; 'triangle', 'square' and 'curve' are used in the domain. The simulation of the droplet spreading behavior on the different roughness texture is simulated very well for impact velocity of 3.0 m/s, 1.5 m/s and 0.5 m/s for all roughness texture.

Higher impact velocity induced the droplet to spread faster and has a bigger diameter. Spreading factor cannot be determined at high impact velocity due to presence of splashing and droplet break up. At impact velocity of 3.0 m/s, splashing occur on all surfaces. Meanwhile at 1.5 m/s the phenomena of splashing is almost absent except on the 'square' surface. The spreading diameter decreased as the impact velocity decreased.

The texture of the substrate also affects the droplet impact behavior. 'Square' surface tends to splash earlier compare to other surfaces and follows by 'triangle', 'curve' and smooth surface. 'Curve' surface which has 'smooth' shape compares to 'triangle' and 'square' which have sharp edges allows the water to spread smoothly.

At low impact velocity, the smooth surface has the highest spreading factor and followed by 'triangle', 'square' and 'curve' surface. Also at low impact velocity, the droplet recoils readily and rapidly, shortening the spreading time.

As for high impact velocities, the droplet spreads without recoils due to kinetic energy exceeding the surface tension forces. It also should be noted that the roughness textures do not show consistent order of spreading factor between the different impact velocities.

In relation to coating coverage on the urea surface, the 'triangle' surface and 'curve' surface resembles closely to uneven surface of urea. To have 'square' surface is almost unlikely. Therefore it can be said that from the simulation, to have the best coating, low velocity of spray should be used to coat the urea which approximately around 0.5 m/s. Also from the simulation result, the coating will be the best if the urea surface has the 'triangle' texture.

5.2 Recommendation

The extension of the future work could be developed if an experiment can be done to validate the results of the simulation. The substrate used for the simulation also can be made to closely resemble urea surface. Since urea is considered to be porous, penetration of the droplet behavior could be included in the simulation. The surface of the flow domain also can be made round shape or on curvature, impersonating the round shape of the urea surface. Also, instead of water, the droplet can be replaced by the material which is actually used for urea coating.

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APPENDIX

APPENDIX 1: MESHING TEXTURE



Figure 36: Different structure of meshing of rough surfaces