# [redacted]

[redacted]

[redacted]

# MODEL OF A DROPLET SPREADING BEHAVIOR ON A TABLET EDGE

By

Mohd Amir Nurasyid Bin Md Said

7704

Dissertation submitted in partial fulfillment of the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

JULY 2009

**Universiti Teknologi PETRONAS**
**Bandar Seri Iskandar**
**31750 Tronoh**
**Perak Darul Ridzuan**

CERTIFICATION OF APPROVAL

**Model of a Droplet Spreading Behavior on a Tablet Edge**

by

Mohd Amir Nurasyid Bin Md Said

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

Approved by,

(Dr. Ku Zilati Ku Shaari)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

July 2009

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.

MOHD AMIR NURASYID BIN MD SAID

**Acknowledgments**

I would like to express my greatest gratitude and appreciation to my advisor Dr. Ku Zilati Ku Shaari for her excellent guidance, patience, generous support, and help. She introduces me to the world of research. She helps me a lot on simulation which is something really new to me. I was fortunate to have a diligent advisor and distinguished teacher like her.

I would like to thank my parents, Md Said Ayob and Zaliha Mohd, whose words of support and guidance are always, be my motivation in finishing my study. Thanks and appreciation for friends and colleague, especially Zulkhaire Ezain Ismail and Mohd Syaiful Hisam Sarno for their full cooperation and constant exchange of information which is very satisfactory throughout the time and proved to be key to optimizing output with regard to the work goals.

For their mutual understanding, motivation and co-operative action, I want to thank all the staff from the Chemical Department of Universiti Teknologi PETRONAS, who treated me like a friend. I enjoyed the effective and professional work very much and I am very happy to have learned so many valuable things under this course.

Finally I would like to dedicate this thesis to all my family members because, this is also their achievement.

## TABLE OF CONTENTS

# CHAPTER 1
# INTRODUCTION

## 1.0 INTRODUCTION

## 1.1 Project Background

Many industrial processing apply the knowledge and concept of droplet spreading behavior in their operations. Spray and coating are the most common operations related this concept to but this may also apply on plant protection, oil recovery from porous rock, lubricant and gluing. Apart from the fundamental problem, many of the practical application require precise knowledge of the rates of the wetting processes because it seems that this process has big influence in droplet spreading behavior. This may explain time taken for the liquid droplet to wet the surface when deposited. M. J. de Ruijter et al. (1999) describe that there are two different types of descriptions of sessile droplet spreading exist: hydrodynamic and molecular kinetic, which differ from each other mostly in the consideration of the dominant dissipation channel. This is basically emphasizes the dissipation due to viscous flow generated in the core of the spreading droplet. Within this approach, a relation between contact angle $\Theta\ (t)$ and the capillary number Ca is derived. This relation, represent a zeroth-order approximation in the expansion power of capillary number yields simple scaling laws determining the time evolution of the contact angle and the droplet's base radius $R(t)$. In case of spreading circular droplet, one finds $R\ (t) \sim t^{1/10}$ and $\Theta\ (t)$ with $t^{-3/10}$ (M. J. de Ruijter et al., 1999). These scaling laws have been examined experimentally and match fairly well with experimental data for most liquid and solid systems (Blake, T. D. et al., 1993).

The second approach, which originates from the molecular kinetic theory, has been tailored to describe the kinetics of wetting phenomena. This approach is in contrast to the hydrodynamic picture because this approach concentrates on the processes occurring in the environment of contact line, which barricade from the attachment of fluid particles to a

solid. Dissipation are ignores in this case due to viscous flows in the core of the liquid droplet. In molecular kinetic approach, the dynamics of the base radius and contact angle $R(t) \sim t^{1/7}$ and $\Theta(t) \sim t^{-3/7}$, respectively.

On the other hand, it has been clearly understood that both types of dissipation do exist simultaneously, and several attempts to work out a combined theory have been made. In particular, a simple way of formulating a combined theory on the basis of the molecular kinetic approach was discussed by Blake, T. D. et al. 1993. By simply adding the barrier created by the liquid or solid attractions to a viscous contribution, the effects of viscous flow can be incorporated into the molecular kinetic approach. In this approach, both two different dissipation channels are taking into account; dissipation due to viscous flows and due to frictional processes.

Standard mechanical approach is adapt to dissipative system in order to describe the time evolution of the droplet, in which the driving force, the gradient of system's Lagrangian function, is balanced by the rate of total dissipation. In this case, the driving force is the loss of the droplet's free energy due to the increase in the base radius.

Despite of this, wettability is also said to be one of the factor effecting droplet spreading behavior. Wetting involves the interaction of a liquid with a solid. It can be the spreading of a liquid over surface, the penetration of a liquid into a porous medium, or the displacement of one liquid by another. It can help to characterize surfaces and to determine solid/liquid interactions. Wettability is most often described by a sessile or resting drop. When a liquid drop is placed in contact with a flat substrate, capillary forces drive the interface spontaneously toward equilibrium. As the drop spreads, the contact angle, $\Theta$, relaxes from its initial maximum of 180° at the moment of contact to its equilibrium angle, $\Theta 0 > 0$ in the case of partial wetting or 0° if the liquid wets the solid completely. The dynamics of spontaneous spreading are usually described at the macroscopic level by an energy balance between a capillary driving force and the hydrodynamic resistance to spreading. The results show the relationships between radius of the base and time or between contact angle and time.

The macroscopic parameters of these master curves are the surface tension and viscosity of the liquid and the volume of the drop. A similar relationship between the spreading rate and viscosity has been obtained using a simplified treatment of the molecular-kinetic theory of viscous spreading given by Cherry and Holmes.

## 1.2 Problem Statement

All over the years, diverse researches and studied on the droplet spreading behavior on surface is been conducted. These researches and studied include theoretical studies, experimentation and numerical methods. The era of modern-advance technologies nowadays encourage and contributes to the rise of more advance researches with aided of software. Computational Fluid Dynamics is one of the examples of integrated software that helps in the development of simulation based research. Most of the research that had been done was mainly to experimentally study the finite volume modeling of droplet impact behavior. However, most of the studied done are mostly concentrated on droplet spreading behavior on the flat surface. Unfortunately, there were fewer researches done to study on the droplet spreading behavior on the edge surface and this was the main reason of this studied is conducted.

This research would examine the droplet spreading behavior on the tablet edge which deputizes the edge surface instead of having flat surface for most of the researches and studied done. An experimental data provided validated in the User Define Function which is produced by Fluent for Fluent Tutorial will be used as reference for the reacting component of this research. Mesh is created by using GAMBIT 2.2.30 in order to simulate this experiment. Through this simulation behavior and pattern of the droplet spreading behavior on created edge mesh is observed. The objective is to predict the short term spreading behavior of a droplet on the edge (known as tablet edge) using a multiphase VOF model which also indicates the maximum spreading diameter resulting from the impact and on different surface roughness theory.

## 1.3 Objective and Scope of Study

The objectives and scope of study of this project are:

1. To study the existing Fluent® model on multiphase volume of fluid (VOF).
2. To model the droplet spreading behavior on a tablet edge using FLUENT 6.2.16 and GAMBIT 2.2.30 software.
3. To model the droplet impact behavior on edge surface with different time steps and surface roughness.

## 1.4 Keywords

Keywords for this project would include: Droplet impact, multiphase VOF

# CHAPTER 2
# LITERATURE REVIEW AND/OR THEORY

## 2.0 LITERATURE REVIEW AND/OR THEORY

This part explain and review related theories with respect to the work in the study of multiphase volume of fluid (VOF) and droplet spreading behavior on edge surface.

## 2.1 Introduction

Wetting is important in many processes both industrial and natural. In many cases, wetting is an essential prerequisite for application, for example in paint films, crop sprays, cosmetics, pharmaceutical tablets and in preparation of suspensions. Both equilibrium and dynamic processes of wetting are important in coatings. The spreading of liquids on substrates is also an important phenomenon as for example in agrochemical applications and in film coatings. The subject of particle/surface adhesion is important in a number of technological and biological applications, examples detergency, paper manufacture, water purification, flotation, fiber manufacture, cell adhesion and attachment, cell separation, bacterial adhesion to tooth surfaces and marine fouling.

Droplet impacting a surface may causing three scenarios to occur; spreading, splashing and rebounding (Yoon, 2006). Figure 1.1 shows these three major droplet impacts. 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 solid, the surface roughness and surface energy are known to have some influence on the behavior of the droplet after the impact.

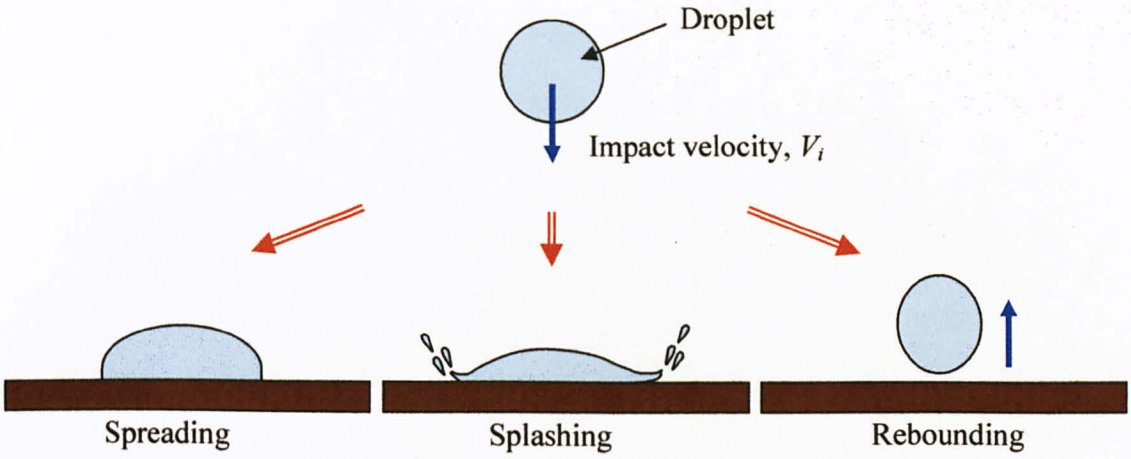



Figure 1: Three major scenario of droplet impact behavior.

A liquid drop can move on a solid surface because of a gradient in wettability along the surface. Such a gradient can be chemically induced (Elwing et al., 1987, Chaudhury & Whitesides, 1992) or can arise from a temperature gradient (Brochard, 1989). The drop will move in the direction of increasing wettability. Available theoretical models are sparse (Greenspan, 1978, Brochard, 1989, Ford & Nadim, 1994) and make several approximations. The approximations include the assumption that the drop wets the surface very well so that the contact angles are small and that the lubrication approximation can be made in simplifying the Navier-Stokes equation. In fact, contact angles in the study of Daniel et al. (2001) are as large as 100°.

Blake & Haynes (1969) developed a kinetic theory model of contact line motion. Their model indicates that a non-hydrodynamic frictional resistance to contact line motion exists. The origin of the frictional resistance is an energy barrier that molecules must cross to move from the liquid drop to available sites on the solid substrate.

This work will look into the relation of water-liquid and air contact angles to the surface where the droplet spreading will occur. The work will be modeled using FLUENT software, version 6.2.16. Findings and result of this work will be discussed at the final section.

## 2.2 Review on fluid dynamic

### 2.2.1 History of fluid dynamic

In 1759 Leonhard Euler published equations of motion for a fluid, applying Newton's second law of motion, which states that the product of mass and acceleration of a body equals the external forces acting on it. Euler's idea to express knowledge about fluid dynamics in the form of partial differential equations was a major breakthrough. A practical shortcoming of his flow model, however, was that it did not consider friction forces.

George Stokes came with more advanced equations in 1845. These equations where already introduced in 1822 by Claude Navier, but only for incompressible fluids. With the freshly introduced equations, today called Navier-Stokes equations, understanding and controlling a large class of fluid flows seemed close at hand. The problem was reduced to the mathematical solution of these basic differential equations.

Although the Navier-Stokes equations meant a considerable theoretical advance, the analytic mathematical solution of the full equations proved one bridge too far. This led to a fragmentation into a large number of simplified equations, derived from Navier-Stokes for special cases, equations which could be tackled analytically, i.e., with pen and paper. However, these different models all described the motion of the same fluid - a theoretically most undesirable situation.

The invention of the digital computer led to many changes. John von Neumann, one of the founding fathers of CFD, predicted already in 1946 that 'automatic computing machines' would replace the analytic solution of simplified flow equations by a 'numerical' solution of the full nonlinear flow equations for arbitrary geometries. Von Neumann suggested that this numerical approach would even make experimental fluid dynamics obsolete.

Von Neumann's prediction did not fully come true, in the sense that both analytic theoretical and experimental research still coexist with CFD. Crucial properties of CFD methods such as consistency, stability and convergence need mathematical study. At present much fundamental research must still be done to increase CFD's accuracy, efficiency and robustness.

### 2.2.2 Computational Fluid Dynamic

Fluid flows play an important role in various equipment and processes in the industry. Flows of air or water are often used for cooling purposes. To localize regions of deficient cooling or to improve the cooling performance of an apparatus insight in the cooling flow pattern is necessary. In general, information about the structure of the flow in a process or an apparatus can be obtained from measurements in experimental test facilities or from flow visualization studies. Although these techniques have proven to be of great importance, there are also limitations and a full picture of the flow field is often hard to obtain in this way. Computational Fluid Dynamics, commonly abbreviated as CFD, is a technique to model fluid flow using a computer simulation. The most fundamental consideration in CFD is how one treats a continuous fluid in a discretized fashion on a computer. One method is to discretize the spatial domain into small cells to form a volume mesh or grid, and then apply a suitable algorithm to solve the equations of motion (Euler equations for inviscid, and Navier-Stokes equations for viscous flow). In addition, such a mesh can be either irregular (for instance consisting of triangles in 2D, or pyramidal solids in 3D) or regular; the distinguishing characteristic of the former is that each cell must be stored separately in memory.

In many instances, other equations are solved simultaneously with the Navier-Stokes equations. These other equations can include those describing species concentration (mass transfer), chemical reactions, heat transfer, etc. More advanced codes allow the simulation of more complex cases involving multi-phase flows (e.g. liquid/gas, solid/gas, liquid/solid), non-Newtonian fluids (such as blood), or chemically reacting flows (such as combustion).

### 2.2.3 Steps in solving CFD problems.

In all of these approaches the same basic procedure is followed.

- During preprocessing
    - The geometry (physical bounds) of the problem is defined.
    - The volume occupied by the fluid is divided into discrete cells (the mesh). The mesh may be uniform or non uniform.
    - The physical modeling is defined - for example, the equations of motions + enthalpy + radiation + species conservation
    - Boundary conditions are defined. This involves specifying the fluid behavior and properties at the boundaries of the problem. For transient problems, the initial conditions are also defined.
- The simulation is started and the equations are solved iteratively as a steady-state or transient.
- Finally a postprocessor is used for the analysis and visualization of the resulting solution.

### 2.2.4 CFD applications

Computational Fluid Dynamics (CFD) has become an indispensable tool in the design, development, evaluation and refinement of new industrial equipment and processes. The use of CFD reduces the development cost of new products and cuts the time to market of these products.

**Product Design**

The ultimate functionality of a product depends on its cost, efficiency, robustness, and acceptance in the commercial market. In products that are developed to improve the environment through energy conservation; fluid-flow, heat and mass transfer plays an important role. CFD now with its multitude capabilities serves as an essential tool for modeling these phenomena in the design of such products.

For instance, in this work CFD is used to model a system that consist of 2 phases which are the tablet edge as primary phase and water droplet as the second phase. Pressure inlet, pressure outlet and wall are the properties that are laid out under primary phase. Primary phase is an essential part that is developed from the beginning of this work by using GAMBIT 2.2.30. Many factors need to be considering while designing primary phase of this work. For example in designing wall, the roughness of the wall surface need to be logic in the sense of the condition of the wall not so rough until the water droplet cannot spread in its normal condition and not so slippery until the water droplet may slip through the wall surface.

Each phase is defined separately from each other because each phase used different material database. Water droplet use $H_2O$ properties in terms of its density, thermal conductivity, viscosity and etc. This is where the multitude capabilities of CFD are being tested.

## 2.3 Volume of fluid (VOF)

In computational fluid dynamics, the volume of fluid method (or in short VOF method) is a numerical technique for tracking and locating the free surface (or fluid-fluid interface). It belongs to the class of 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.

The VOF method is known for its ability to conserve the "mass" of the traced fluid, also, when fluid interface changes its topology, this change is traced easily, so the interfaces can for example join, or break apart.

The method is based on the idea of so called fraction function $C$. It is defined as the integral of fluid's characteristic function in the control volume (namely volume of a computational grid cell). Basically, when the cell is empty (there's no traced fluid inside) value of $C$ is zero, if cell is full, we have $C = 1$, and when the interphasal interface cuts the

cell, then $0 < C < 1$. C is a discontinuous function, its value jumps from 0 to 1 when the argument moves into interior of traced phase.

The fraction function $C$ is a scalar function, and while the fluid moves with velocity $\mathbf{V} = (u(x, y, z), v(x, y, z), w(x, y, z))$ (in three-dimensional space $\mathbf{R}^3$) every fluid particle retains its identity, i.e. when a particle is a given phase, it doesn't change the phase - like a particle of air, that is a part of air bubble in water remains air particle, regardless of the bubble movement (actually, for this to hold, we have to disregard processes such as dissolving of air in water). If that is so, then the substantial derivative of fraction function $C$ needs to be equal to zero:

$$\frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C = 0.$$

This is actually the same equation that has to be fulfilled by the level set distance function $\varphi$.

There are various means to solve this equation. It cannot be solved directly easily, since $C$ is discontinuous, nevertheless such attempts have been performed. But most popular approach to the equation is the so called geometrical reconstruction, originating in the works of Hirt and Nichols.

In the VOF models, Geo-Reconstruct method is used to define the multiphase parameters. This is the most accurate interface-tracking scheme and is recommended for most transient VOF calculation. Using this method, the interface between fluids is represented using a piecewise-linear interface calculation (PLIC), which assumes that the interface has a linear slop within each cell. Courant number is set to be at 0.25 which is the condition for convergence while solving certain partial different equations numerically. Time step must be less than a certain time in many explicit time marching computer simulations.

### 2.3.1 Surface tension

The effects of surface tension along the interaction interface between two phases are also included in the VOF model. Surface tension is caused by the attraction between the liquid's molecules by various intermolecular forces. In the bulk of the liquid, each molecule is pulled equally in every direction by neighbouring liquid molecules, resulting in a net force of zero. At the surface of the liquid, the molecules are pulled inwards by other molecules deeper inside the liquid and are not attracted as intensely by the molecules in the neighbouring medium. Therefore, all of the molecules at the surface are subject to an inward force of molecular attraction which is balanced only by the liquid's resistance to compression, meaning there is no net inward force. However, there is a driving force to diminish the surface area. Thus the liquid squeezes itself together until it has the locally lowest surface area possible.

Another way to view it is that a molecule in contact with a neighbour is in a lower state of energy than if it weren't in contact with a neighbour. The interior molecules all have as many neighbours as they can possibly have. But the boundary molecules have fewer neighbours than interior molecules and are therefore in a higher state of energy. For the liquid to minimize its energy state, it must minimize its number of boundary molecules and must therefore minimize its surface area.

As a result of surface area minimization, a surface will assume the smoothest shape it can; mathematical proof that "smooth" shapes minimize surface area relies on use of the Euler–Lagrange equation. It was developed by Swiss mathematician Leonhard Euler and Italo-French mathematician Joseph Louis Lagrange in the 1750s. A differentiable functional is stationary at its local maxima and minima, the Euler–Lagrange equation is useful for solving optimization problems in which, given some functional, one seeks the function minimizing (or maximizing) it.

The Euler–Lagrange equation is an equation satisfied by a function $q$ of a real argument $t$ which is a stationary point of the functional:

$$S(q) = \int_a^b L(t, q(t), q'(t))\,\mathrm{d}t$$

where:

$q$ is the function to be found:

$$\begin{aligned} q\colon [a, b] \subset \mathbb{R} &\to X \\ t &\mapsto x = q(t) \end{aligned}$$

such that $q$ is differentiable, $q(a) = x_a$, and $q(b) = x_b$;

$q'$ is the derivative of $q$:

$$\begin{aligned} q'\colon [a, b] &\to T_{q(t)}X \\ t &\mapsto v = q'(t) \end{aligned}$$

$TX$ being the tangent bundle of $X$ (the space of possible values of derivatives of functions with values in $X$);

$L$ is a real-valued function with continuous first partial derivatives:

$$\begin{aligned} L\colon [a, b] \times TX &\to \mathbb{R} \\ (t, x, v) &\mapsto L(t, x, v). \end{aligned}$$

The Euler–Lagrange equation, then, is the ordinary differential equation

$$L_x(t, q(t), q'(t)) - \frac{\mathrm{d}}{\mathrm{d}t} L_v(t, q(t), q'(t)) = 0.$$

where $L_x$ and $L_v$ denote the partial derivatives of $L$ with respect to the second and third arguments, respectively.

If the dimension of the space $X$ is greater than 1, this is a system of differential equations, one for each component:

$$\frac{\partial L(t, q(t), q'(t))}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L(t, q(t), q'(t))}{\partial v_i} = 0 \quad \text{for } i = 1, \ldots, n.$$

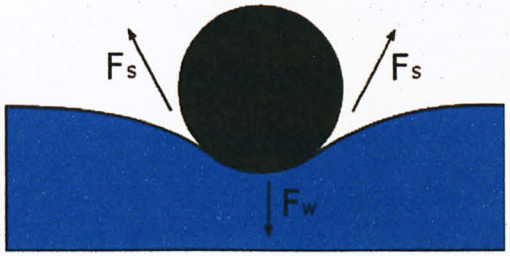



Figure 2: Relation of weight and surface tension.

Diagram shows, in cross-section, the relation between weight and surface tension. Its weight, $F_w$, depresses the surface, and is balanced by the surface tension forces on either side, $F_s$, which are each parallel to the water's surface at the points where it contacts the needle. Notice that the horizontal components of the two $F_s$ arrows point in opposite directions, so they cancel each other, but the vertical components point in the same direction and therefore add up to balance $F_w$.

Throughout this work, water droplet is the major concern is studying the droplet spreading behavior on edge. Thus, the radius of water droplet is said to be one of the important part in this study. Radius will be closely related to the pressure exerted on the surface.

The table below shows how the internal pressure of a water droplet increases with decreasing radius. For not very small drops the effect is subtle, but the pressure difference becomes enormous when the drop sizes approach the molecular size.

| **$\Delta p$ for water drops of different radii at standard temperature and pressure.** | | | | |
|---|---|---|---|---|
| Droplet radius | 1 mm | 0.1 mm | 1 μm | 10 nm |
| $\Delta p$ (atm) | 0.0014 | 0.0144 | 1.436 | 143.6 |

Table 1: Radius-pressure relation.

### 2.3.2 Wall adhesion

Wall adhesion is the cohesive forces existing between the wall and a fluid. The contact angle that the fluid and wall produced can determine the local curvature that is used to adjust body force in surface tension calculation.

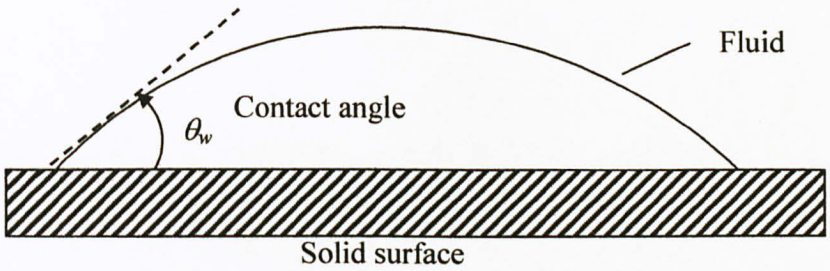



Figure 3: Schematic diagram showing the contact angle between phases.

Both k- omega models (std and sst) are available as low-Reynolds-number models as well as high-Reynolds-number models. The wall boundary conditions for the k equation in the k- omega models are treated in the same way as the k equation is treated when enhanced wall treatments are used with the k- epsilon models.

This means that all boundary conditions for:

- Wall-function meshes will correspond to the wall function approach.
- Fine meshes, the appropriate low-Reynolds-number boundary conditions will be applied.

That means:

If the Transitional Flows option is enabled in the Viscous Model panel, low-Reynolds-number variants will be used, and, in that case, mesh guidelines should be the same as for the enhanced wall treatment. (y+ at the wall-adjacent cell should be on the order of y+ = 1.

However, a higher y+ is acceptable as long as it is well inside the viscous sub layer (y+ < 4 to 5).)

If Transitional Flows option is not active, then the mesh guidelines should be the same as for the wall functions. (For wall functions, each wall-adjacent cell's centroid should be located within the log-law layer, 30 < y+ < 300. A y+ value close to the lower bound **y+ = 30** is most desirable.)

# CHAPTER 3
# METHODOLOGY/PROJECT WORK

## 3.0 METHODOLOGY/ PROJECT WORK

There are basically two methods in discovering the droplet impact studies; by experiment and modeling. This work is more interested on the modeling method using FLUENT 6.2.16 software. Experimental method is more to lab work where high speed camera allowing a frame rate of 2000 images/s is used. Precise syringe pump for forming millimeter sized drops and ink-jet-print-heads for ejecting drops are usually used for cases where micro droplet sized is performed. The size of the big drops can be tuned by changing the needle and those used in this work allowed forming drops between 1.7 and 2.3 mm (Morougou-Candoni N. et al., 1999). The manipulation of the drive waveform allows ejecting small sized drops with velocities varying between 1 and 7 m/s. (Desie G. et al., 2003).

Kim et al. (2003) studied the dynamics of micro-droplets. Experiment was run using 100 μm sized water droplet with impacting velocity on flat surface of 10 m/s. Drop generation system was used to produce a stream of mono-sized droplets and the images of spreading behavior of the droplet were obtained using a double-flash photography technique.

In other cases, Roux and Copper-White (2004) studied the dynamics of water droplets impacting on a glass surface using a high-speed camera. Experiments were performed with a wide range of impact velocities. This study concluded that spreading can be divided into two types of behavior, namely, low impact velocity and high impact velocity. Low impact velocity and high impact velocity explain the condition of droplets spreading behavior after impacting glass surface.

These are some examples of droplet impact study through experimental approach. However, experimental approach is not the concern in this work. Modeling approach will be use throughout this work.

### 3.1 Modeling – FLUENT:

Computational fluid dynamics (CFD) is one of the branches of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the millions of calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. The fundamental basis of almost all CFD problems is the Navier-Stokes equations, which defined any single-phase fluid flow. The Navier-Stokes equations were named after Claude-Louis Navier and George Gabriel Stokes. These equations describe the motion of fluids (liquids and gasses).

In this work, FLUENT software, version 6.2.16, was used to model the spreading behavior of a liquid droplet. Mesh geometries used in this work was created using GAMBIT software, version 2.2.30. It is important to make sure that mesh created contains equivalent nodes at every side in order to get a balance and accurate calculation. Mirror effect is suggested to be used in this work to obtain equal computational time. A 2-mm droplet having properties of water ($H_2O$) are patched on the mesh surface.

### 3.2 Model development

There are three major processes in model development process. The first is the most crucial part which is the mesh development in GAMBIT software. Accuracy in making sure that every side of model is having equal nodes is very important. This will help to determine the accuracy of modeling on study area.

Next steps are to set up the solver and properties. This is done at both software; FLUENT 6.2.16 and GAMBIT 2.2.30. Boundaries conditions is one of the example of properties that need to be set up.

The final steps are the model initialization and solution monitoring. Less work is required in this part since most of the solver and properties has been set up. Following are the summary of steps development in FLUENT model for this work.

1. Mesh development in GAMBIT
2. Solver and properties set up
3. Model initialization and solution monitoring

## 3.3 Methodology

The methodology is as follow (Fluent Software Training, 2001)

- Problem Identification and Pre-Processing
  - i. Modelling goals:
    This is the part which decision on what results are actually is looking for
  - ii. Domain of the model:
    In this part, boundary conditions are decided to be used throughout this work.
  - iii. Create grid:
    Type of grid is chosen to be used in this step.
- Solver Execution
  - iv. Setting up the numerical method
    Multiphase VOF is the area of study for this work.
  - v. Computing and monitoring the solution
- Post Processing
  - vi. Examining the result
  - vii. Considering on optimizing the model

### 3.3.1 Mesh development

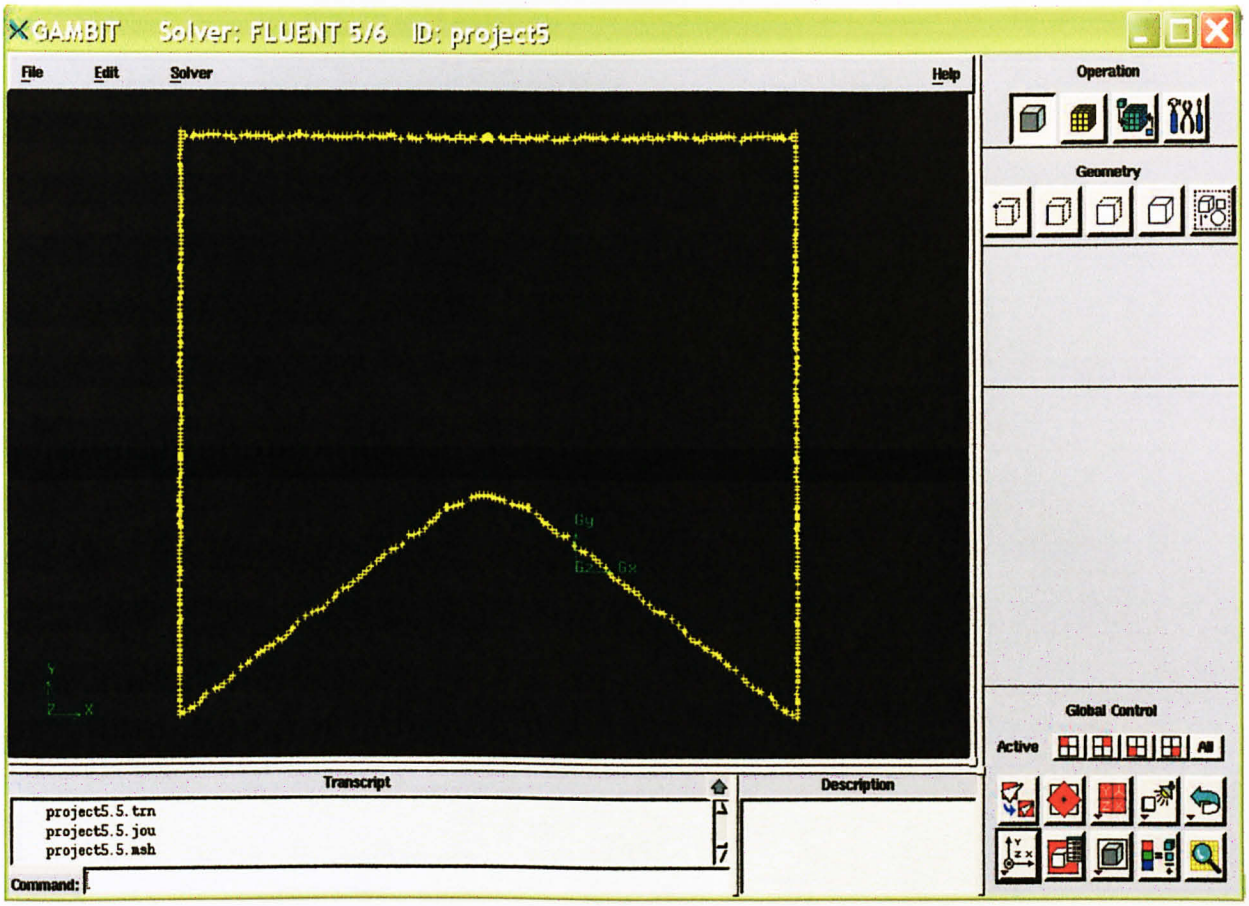



Figure 4: Mesh is created at the first stage using software GAMBIT 2.2.30.

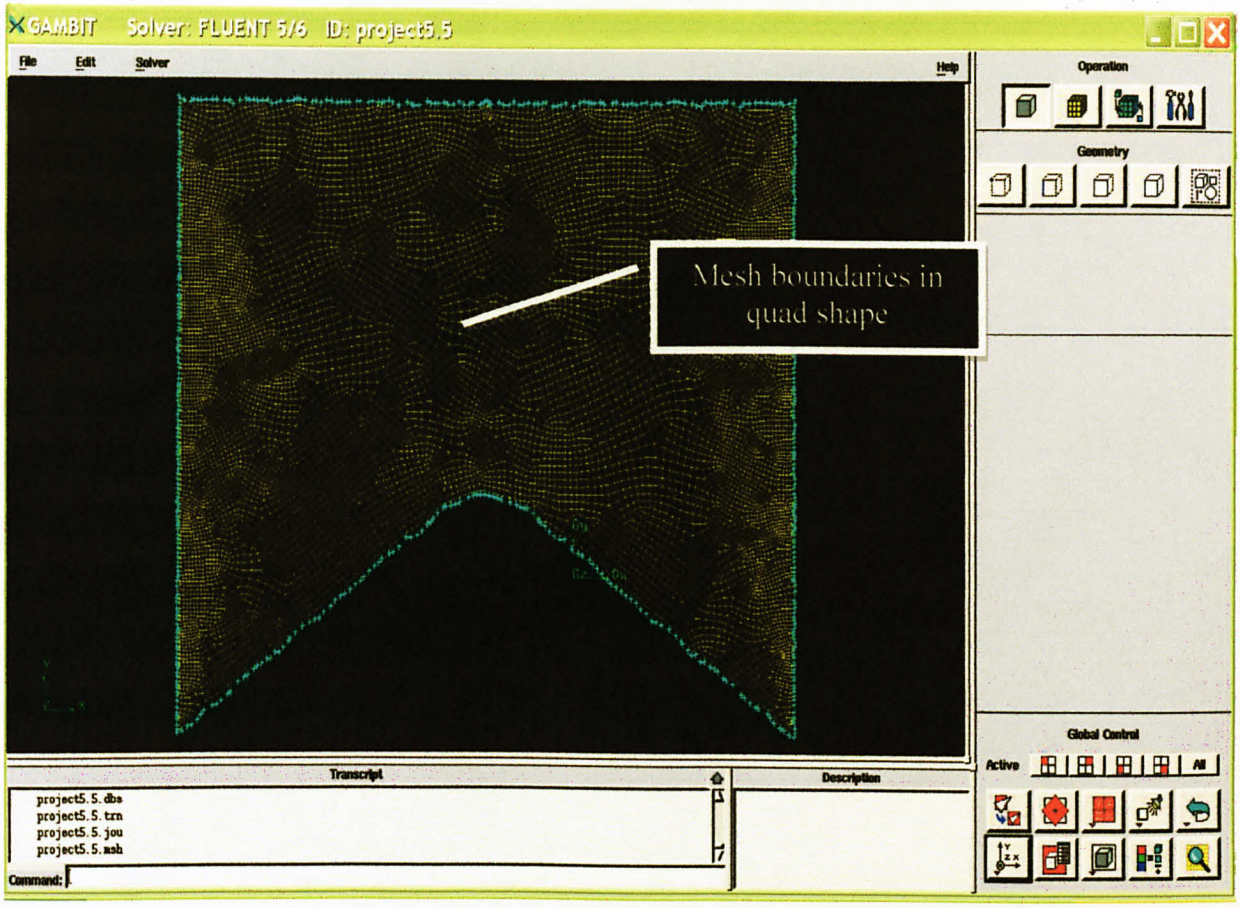



Figure 5: Quad shape is being chosen to show the mesh grid.

In mesh development, GAMBIT 2.2.30 software is used. Shape that is created as figure above represents the area of interest in this work, which is the tablet edge. The coordinate of the point surface need to be verifying as to start the mesh development. Point surface coordinate for mesh used in this work are x= -2.03787e-06 and y= 1.572627e-06. The reason why the point surfaces coordinates need to be know is to make mesh development and point tracing easier else future mesh development might faced problem in terms of finding the coordinate of nodes.

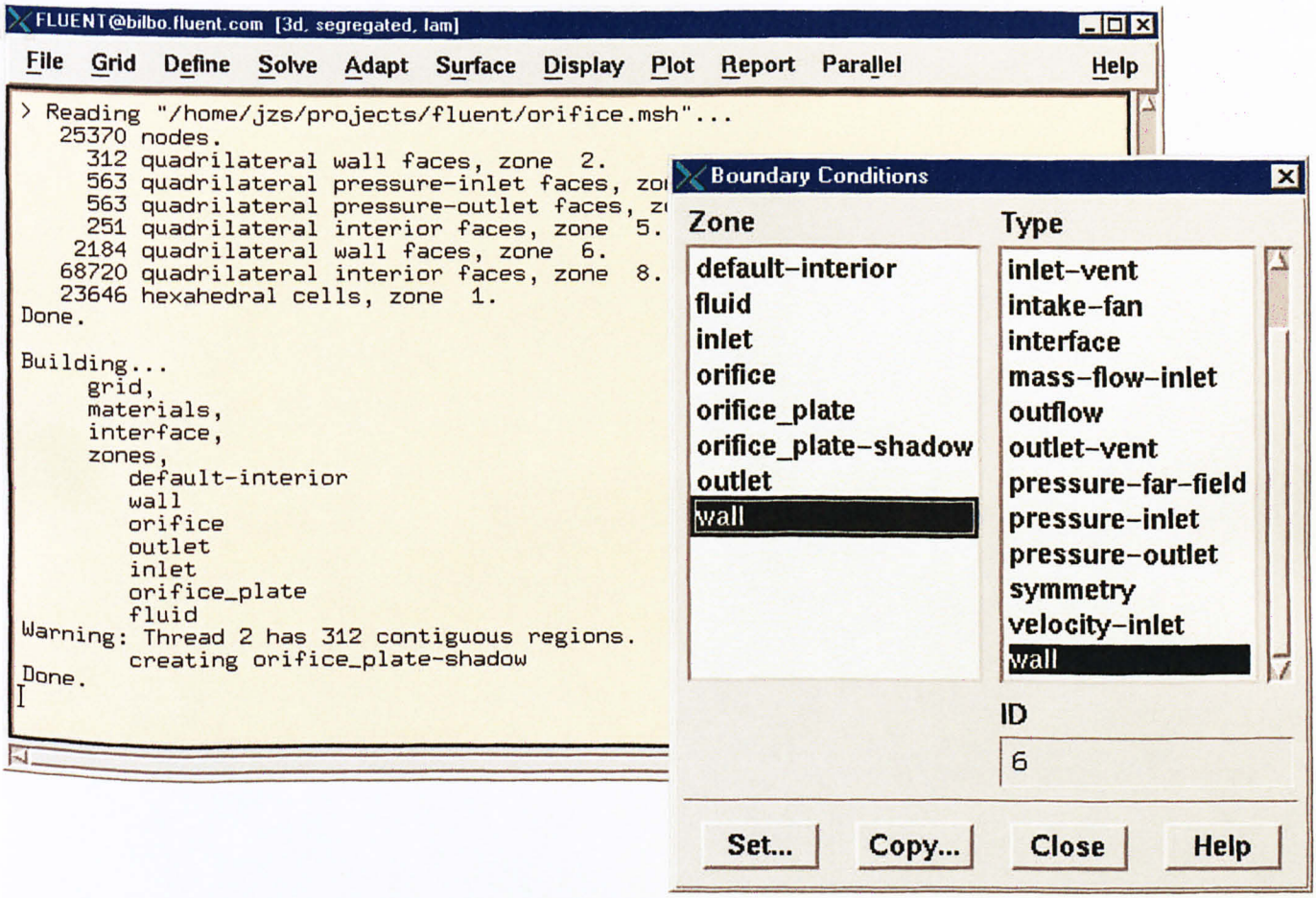



Figure 6: Reading mesh zone on FLUENT 6.2.16 software.

### 3.3.2 Scaling Mesh and Units

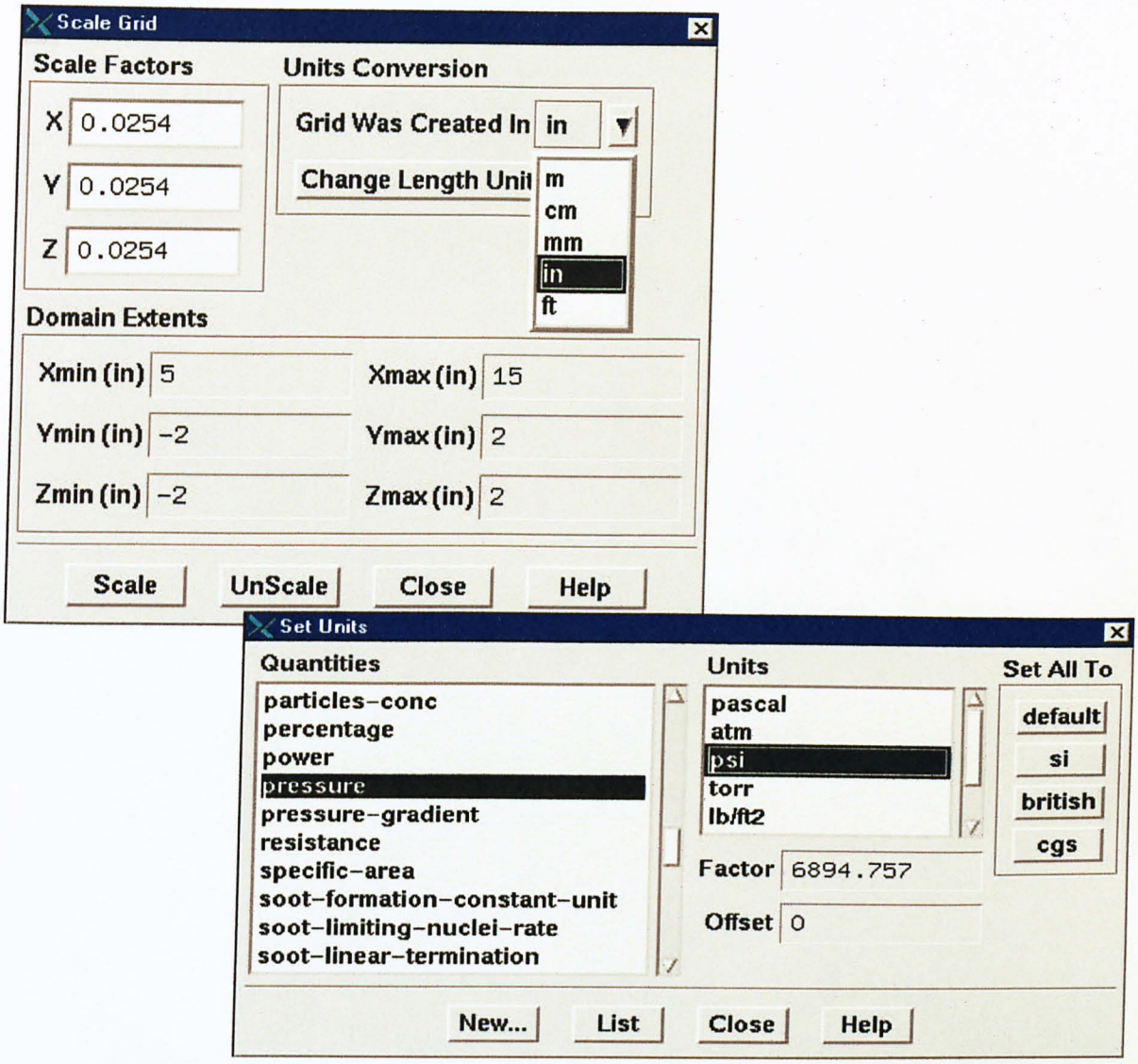



Figure 7: Scaling mesh and unit.

All physical dimensions are initially assumed to be in millimeters because the droplet used for this work is in nano size which is 2mm. So this is important that this work used small dimension to indicate the material precisely otherwise inaccurate data will be obtained throughout this work.

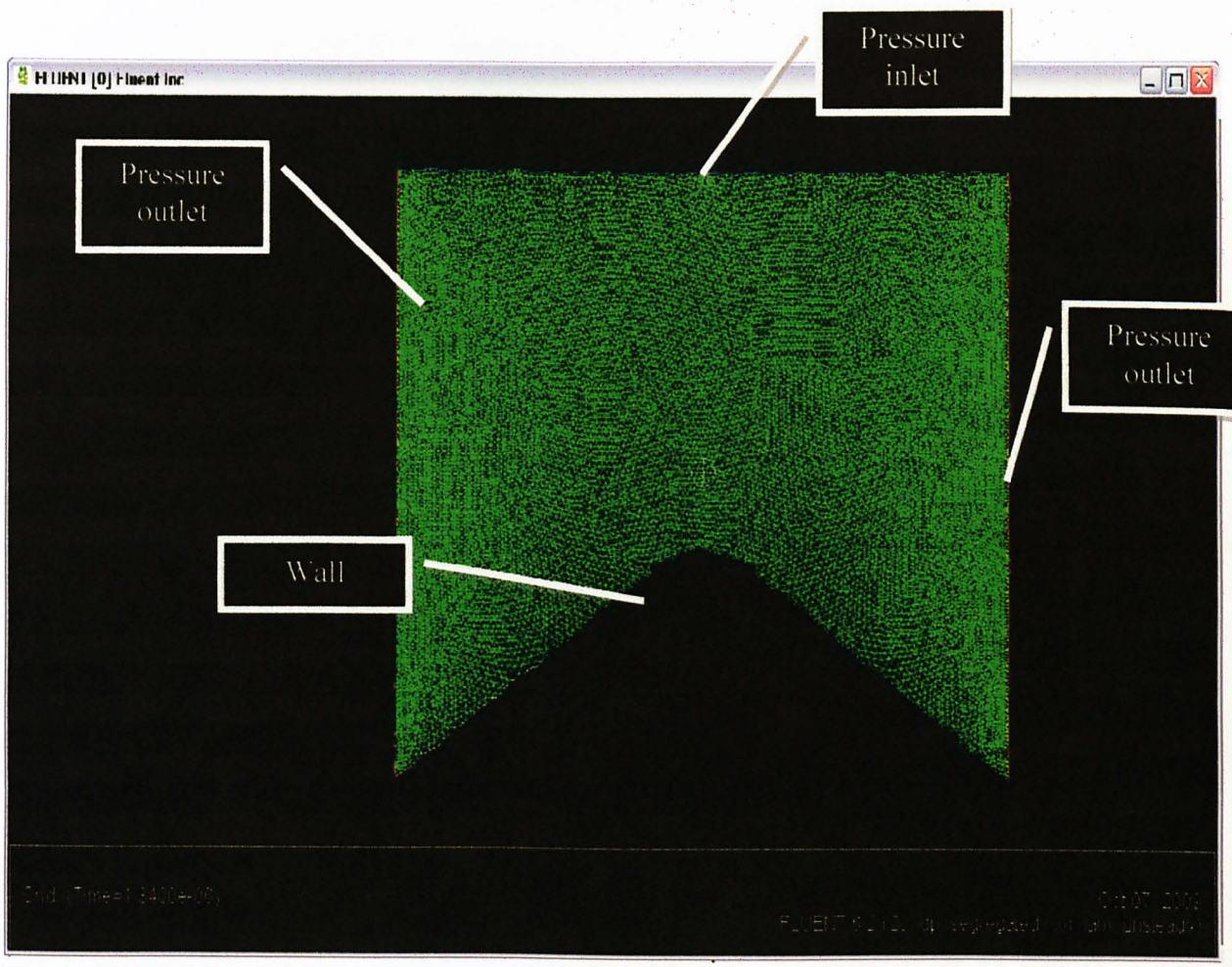



Figure 8: Complete mesh with defined properties.

Both left and right side of the model represent the pressure outlet and top most boundaries represent the pressure inlet. Pressure coming in and going out is set to be constant at 1atm. Wall is actually an illustration of the tablet edge where the droplet impact will take place. Boundary data required depends on physical models selected. General guidelines:

- Select boundary location and shape such that flow either goes in or out.
- Not necessary, but will typically observe better convergence.
- Should not observe large gradients in direction normal to boundary

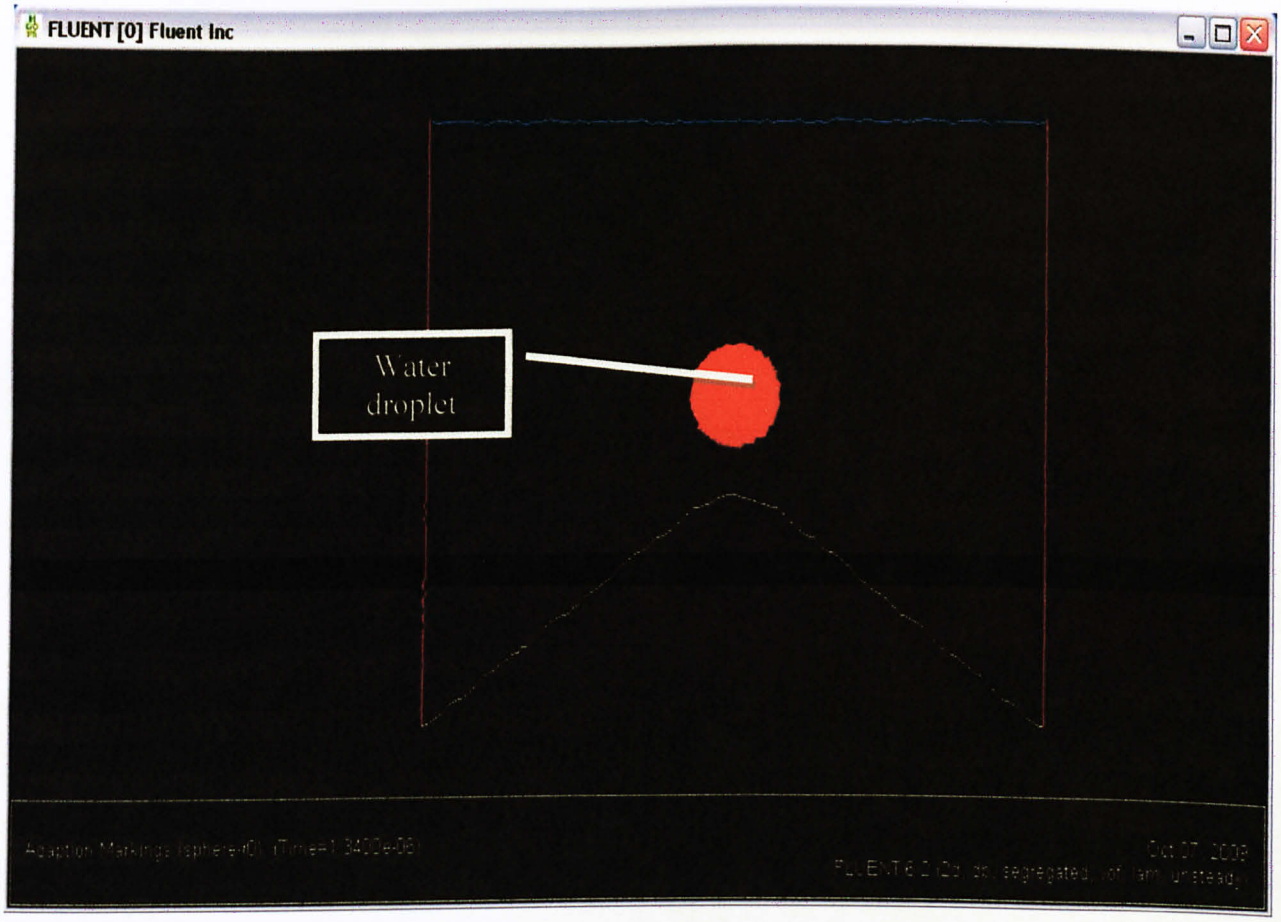



Figure 9: Circle at the top of edge represents the water droplet.

Water droplet is patched as a second phase on the mesh surface. The droplet velocity is set to be at constant of 0.5m/s.

### 3.4 Gantt chart

| No. | Detail/ Week | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Briefing on FYP | ■ | | | | | | | | | | | | | |
| 2 | Selection of Project Topic | ■ | ■ | | | | | | | | | | | | |
| 3 | Preliminary Research Work | | ■ | ■ | ■ | | | | | | | | | | |
| 4 | Proposal Submission to Supervisor | | | ■ | | | | | | | | | | | |
| 5 | Submission of Preliminary Report | | | | ■ | | | | | | | | | | |
| 6 | Project Work | | | | ■ | ■ | ■ | ■ | | | | | | | |
| 7 | Submission of Progress Report | | | | | | | ■ | | | | | | | |
| 8 | Seminar (optional) | | | | | | | | ■ | ■ | | | | | |
| 9 | Project Work | | | | | | | | ■ | ■ | ■ | ■ | ■ | ■ | ■ |
| 10 | Submission of Interim Report Final Draft | | | | | | | | | | | | | | ■ |

■ Process

# CHAPTER 4
# RESULTS AND DISCUSSION

## 4.0 RESULTS AND DISCUSSION

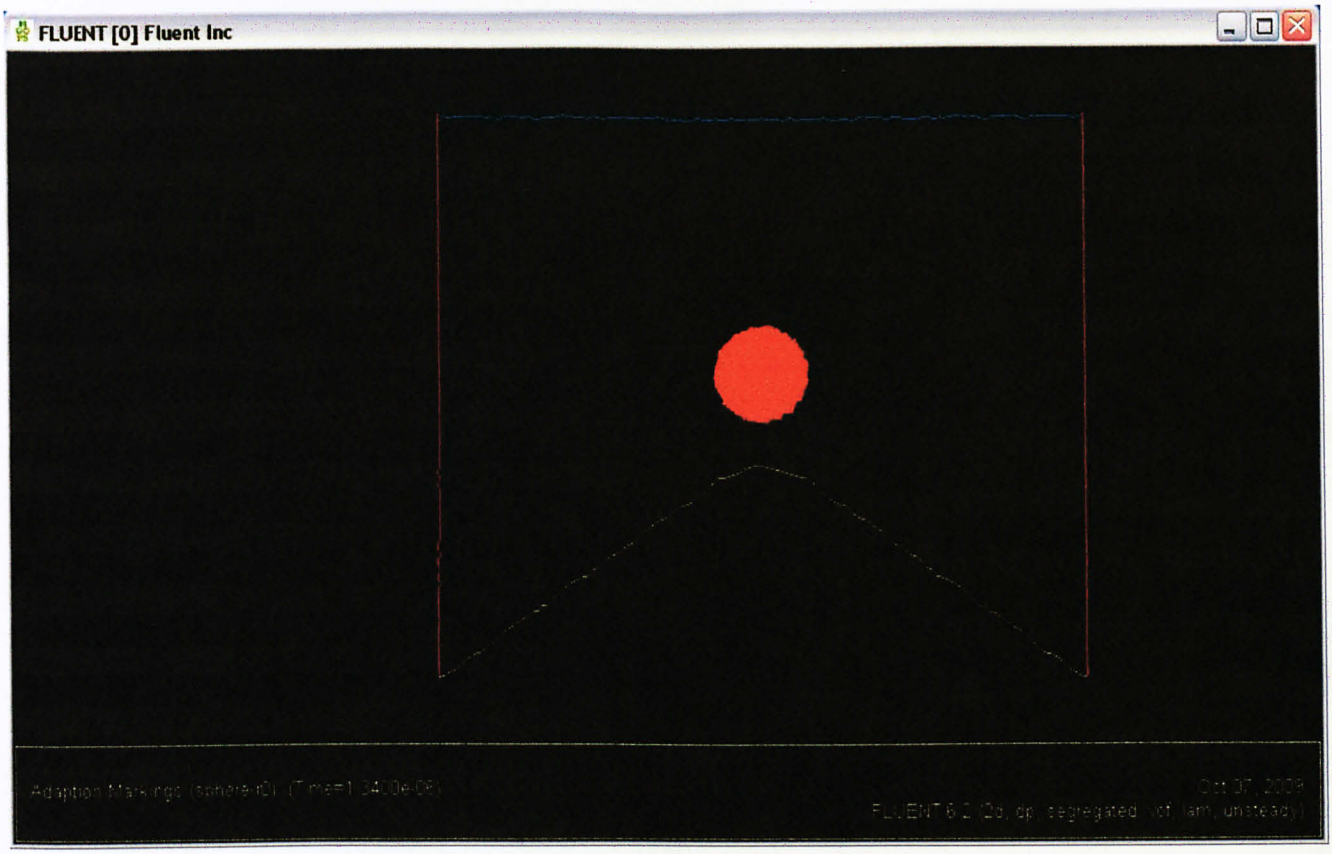



Figure 10: Droplet initial condition.

Figure above is the initial condition of single water droplet before impacting tablet edge while figure below is the condition of a single water droplet after impacting tablet edge. Initially, water droplet is patched up above the inclined tablet edge before it is simulate to impact the tablet edge with velocity -0.5m/s. Laminar condition is used for this simulation. Properties of $H_2O$ such as the density, thermal conductivity and viscosity are used to define water droplet in this work. Under the wall adhesion property, surface tension coefficients used in this work is set to constant at 73.5dyn/cm. Surface tension is a

property of the surface of a liquid. It is what causes the surface portion of liquid to be attracted to another surface, such as that of another portion of liquid. Applying Newtonian physics to the forces that arise due to surface tension accurately predicts many liquid behaviors that are so commonplace that most people take them for granted. Applying thermodynamics to those same forces further predicts other more subtle liquid behaviors. Surface tension has the dimension of force per unit length, or of energy per unit area.

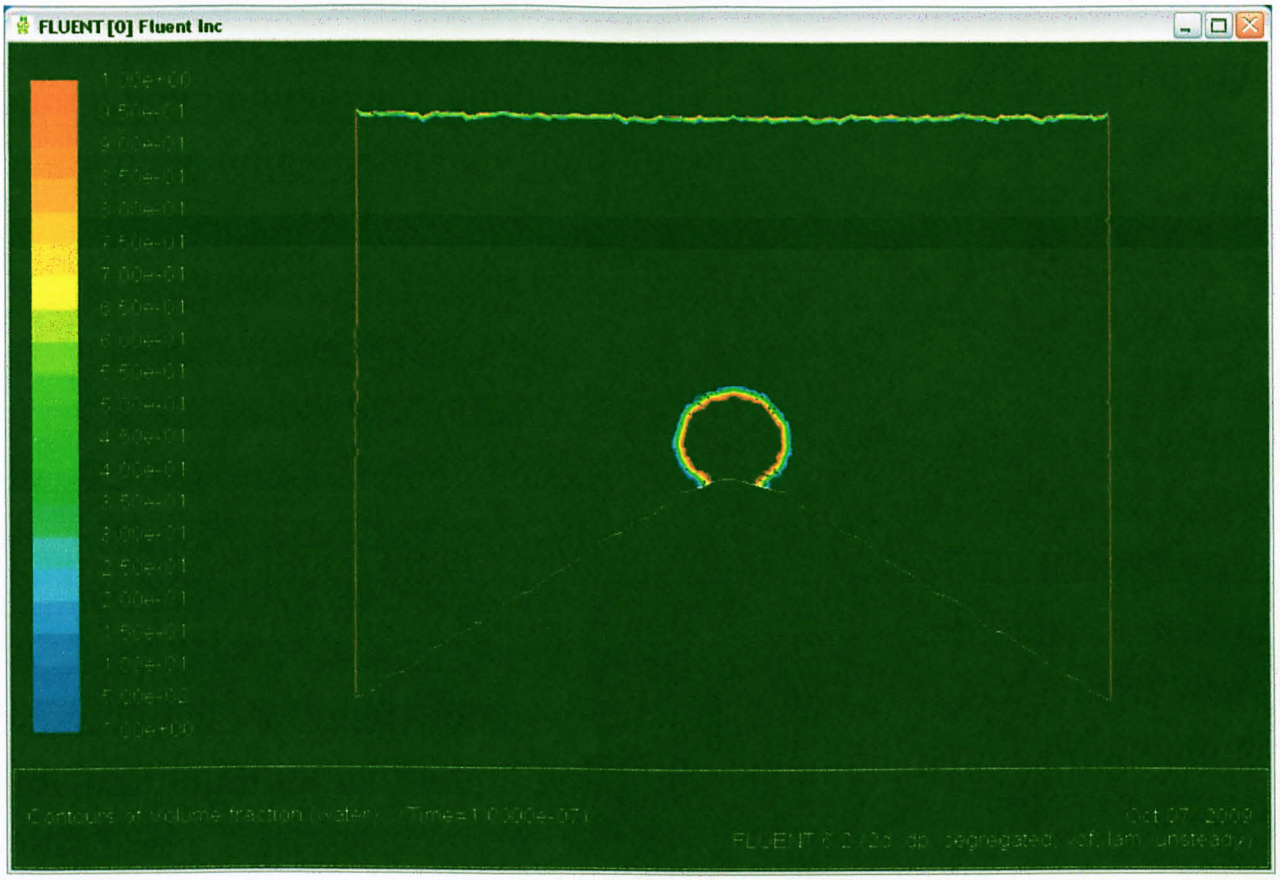



Figure 11: Droplet impacting tablet edege.

After running this simulation, it is believed that the wall surface roughness is the main reason for the water droplet to stick at the top of the edge after impacting surface. It is defined here in this simulation for the wall roughness to have a constant roughness of 0.5. Stationary wall is used in this work with no-slip shear condition.

Contact angles for water and air used in this work is 175°. It is set to be constant throughout this work. The contact angle is the angle at which a liquid/vapor interface

meets the solid surface. The contact angle is specific for any given system and is determined by the interactions across the three interfaces. Most often the concept is illustrated with a small liquid droplet resting on a flat horizontal solid surface. The shape of the droplet is determined by the Young Relation. The contact angle plays the role of a boundary condition. The contact angle is not limited to a liquid/vapor interface; it is equally applicable to the interface of two liquids or two vapors.

The computational modeling parameters were chosen after verification and validations. All the results presented in this study are with the computational modeling parameters shown in Table 2.

| **Computational parameters** | **Setting of the computational parameters** |
|---|---|
| Mesh type | Quadrilateral |
| Solver | Unsteady |
| Discretization | Pressure (body force weighted), momentum (second order), gravity |
| Pressure-velocity coupling | PISO Ferzieger and Peric (1996) |
| VOF parameters | Geometric reconstruction Youngs (1982) |
| Time step | Minimum=1e-08s |

Table 2: Modeling parameters.

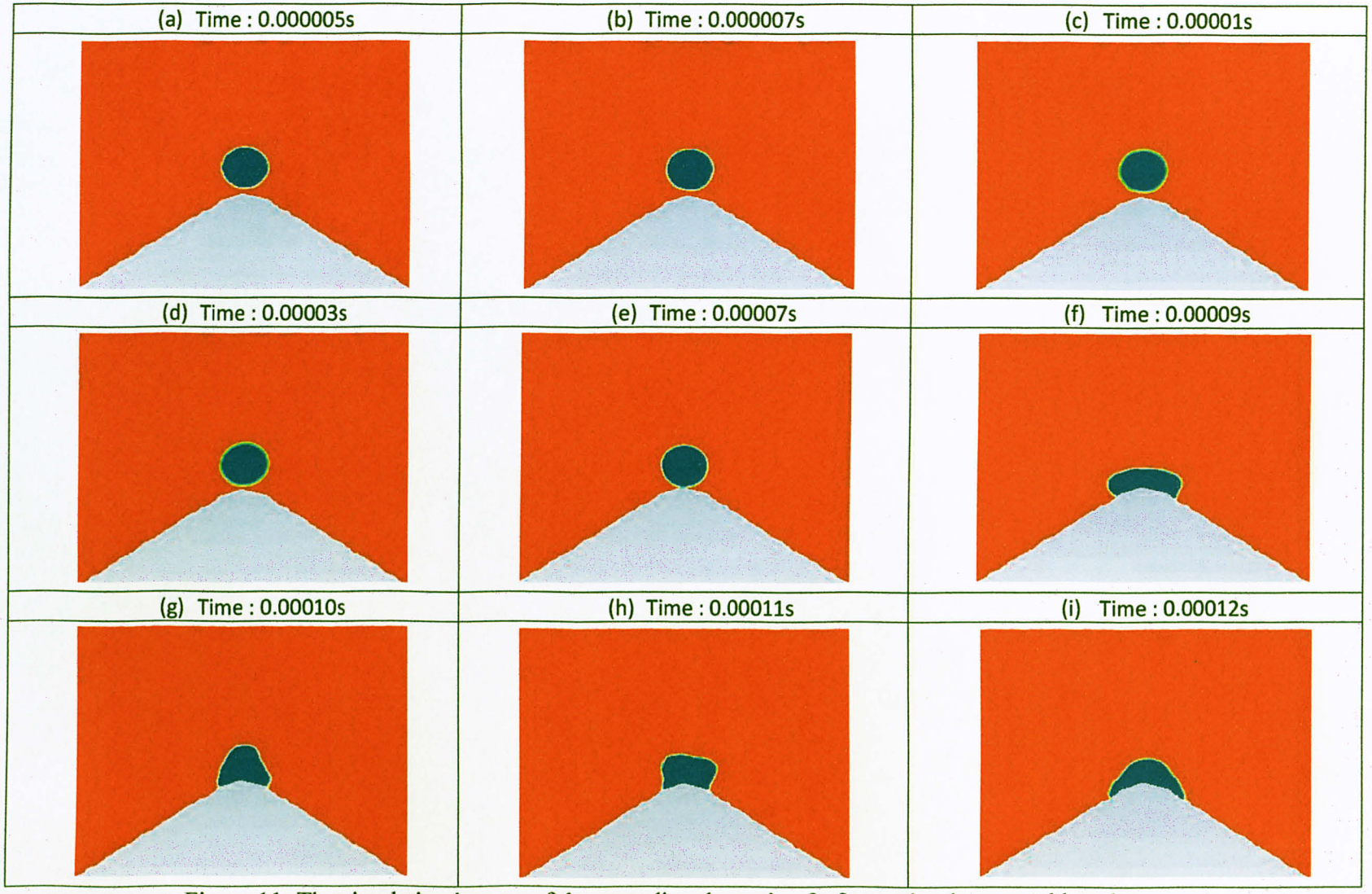
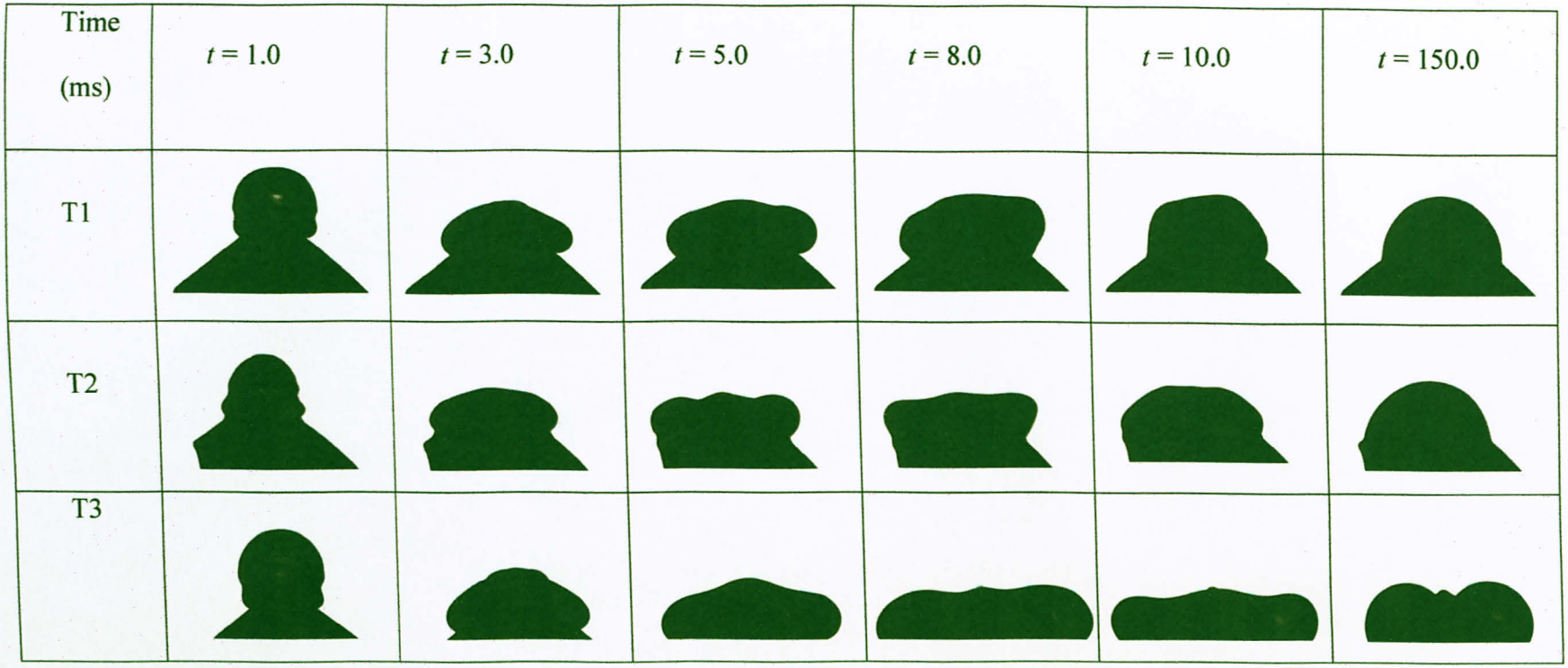


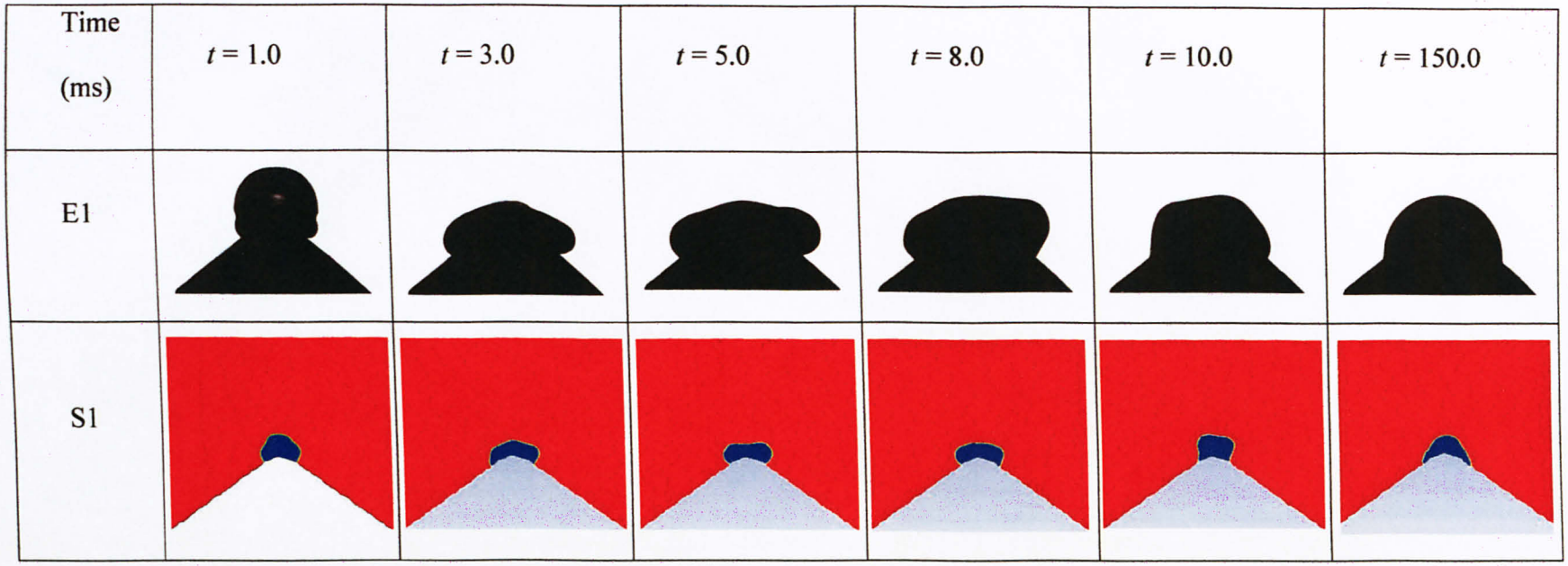

Figure 11: The simulation images of the spreading dynamic of a 2-mm droplet on a tablet edge.




T1 = rough, non-coated tablet T2 = rough, coated tablet T3 = smooth, non-coated tablet

Figure 12: The experimental images of a 2-mm droplet after impacting tablet edge.

These droplet behaviors were obtained through experiment (Ku Zilati Ku Shaari, 2007). Three different edge surface conditions were used during the experiment to look into the effect of surface roughness to the spreading behavior. However, in this study surface roughness is put into constant and is considered as rough.




E1: Proven by experiment.
S1: Obtained from simulation.

Figure 13: Comparison between experimental and simulation figure by using the same time step.

Above figures shows the comparison of droplet spreading behavior through two different method; experiment and simulation. It shows that the behaviors of droplet spreading are the same at same time.

# CHAPTER 5
# CONCLUSION AND RECOMMEDATION

## 5.0 CONCLUSION AND RECOMMEDATION

### 5.1 Conclusion

In this paper, the collision dynamics of single drop impinging on a tablet edge have been detailed and modeled. In the case of single drop with 2mm size impacts occurring at velocity -1m/s shows the accumulation of water droplet on the top of the tablet edge at first than it showed all scenarios of major spreading behavior; spreading, splashing and rebounding. More sophisticated numerical simulation is necessary for impacts at high Reynolds numbers where the profiles are quite intricate and further work is still needed in that area. Low velocity drop onto drop axisymmetric collisions can be split into three phases: a latency period during which the drop stays pinned on the substrate and finally a spreading phase with the maximum diameter given by energetic considerations.

### 5.2 Future Work

*To simulate the mixing process with different surface roughness and water-surface contact angles.*

## References


Blake, T. D. & Haynes, J. M., (1969), "Kinetics of liquid/liquid displacement"., Journal of Colloid and Interface Science 30, 421-423.

Blake, T. D. and Haynes, J. M.*J., "Colloid Interface Sci". (*1969), *30*, 421.

Bussman, M., Mostaghimi, J. and Chandra, S., (1999), "On a three-dimensional volume tracking model of droplet impact", *Physics of Fluids*, 11(6), 1406-1417.

Chaidron, G., Soucemarianadin, A. and Attané, P., (1999), "Study of impact of drops onto solid surfaces", *International Conference on Digital Printing Technologies.*

Damien Vadillo, Guido Desie, Arthur Soucemarianadin, (August 2004), *Laboratoire des Ecoulements Géophysiques et Industriels (LEGI),* "Spreading Behavior of Single and Multiple Drops"

de Gennes, P. G., (1985), "Wetting: Statics and dynamics", Reviews of Modern Physics 57,827-863.

de Ruijter, M. J., Blake, T. D., & De Coninck, J., (1999), "Dynamic wetting studied by molecular modeling simulations of droplet spreading", Langmuir 15, 7836-7847.

Fluent Software Training, Fluent Incorporated. 2001

Fluent Software Tutorial Guide, Fluent Incorporated 2006

Fluent Software User Guide, Fluent Incorporated 2006

Fukai, J., Shiiba, Y., Yamamoto, T., Miyatake, O., Poulikakos, D., Megaridis, C. M., and Zhao, Z., (1995), "Wetting effects on the spreading of a liquid droplet colliding with a at surface: Experiment and modeling", *Physics of. Fluids*, **7**, 236-247.

Gambit Software Tutorial Guide, Fluent Incorporated 2001.

Hirt, C.W.; Nichols, B.D. (1981), "Volume of fluid (VOF) method for the dynamics of free boundaries", *Journal of Computational Physics* **39** (1),

Hitoshi Fujimoto, Tomoyuki Ogino, Hirohiko Takuda and Natsuo Hatta, (December 200), "Collision of a droplet with a hemispherical static droplet on a solid", *Department of Science and Technology, Graduate School of Energy Science, Kyoyo University, Yoshida-Honmachi, Sakyo-ku, Kyoto, Japan.*

J. B. McLaughlin, Sp. S. Saravanan, N. Moumen, and R. S. Subramanian, (1999), "Modeling of Drop Motion on Solid Surfaces with Wettability Gradients", *Department of Chemical Engineering, Clarkson University.*

Ku Zilati Ku Shaari, Dr. Richard Turton, Chair, Dr. Charter D, Stinespring, Dr. Wade Huebsch, Dr. Paula Stout, Dr. Eugene Cilento, (2007), "Coating uniformity on a pharmaceutical tablet: An experimental study and finite volume modelling of droplet impact behavior", *Department of Chemical Engineering, Morgantown, West Virginia.*

M. J. de Ruijter, J. De Coninck, and G. Oshanin, (August 1998), "Droplet Spreading: Partial Wetting Regime Revisited", *Centre de Recherche en Mode'lisation Mole'culaire, Universite' de Mons-Hainaut*

Portela L.M. and Oliemans R.V.A., (2006), "Possibilities and Limitations of Computer Simulations of Industrial Turbulent Dispersed Multiphase Flows", *Delft University of Technology, Netherlands, Springer.*

Shanahan, M. E. R.; de Gennes, P. G., *"Adhesion"*, Allen, K. W., Ed.; Elsevier Applied Science: London, (1987); p 71.

Sikalo, S., Tropea, C. and Gani, E.N., (2005), "Impact of droplets onto inclined surfaces", *Journal of Colloid and Interface Science*, **286**, 661-669.

T. D. Blake and A. Clarke, *Kodak European Research, Kodak Limited, Harrow HA1 4TY, U.K.,* J. De Coninck and M. J. de Ruijter, *Research Center for Molecular Modelling, Faculte' des Sciences, Universite' de Mons-Hainaut,* (January 1997), "Contact

Angle Relaxation during Droplet Spreading Comparison between Molecular Kinetic Theory and Molecular Dynamic".

Toivakka, M., (2003), "Numerical Investigation of droplet impact spreading in spray coating of paper", *Spring Advanced Coating Fundamentals Symposium*.

Vivek V Ranade,, (2002), "Computational Flow Modelling for Chemical Process Engineer", *Academic Press*.

Yoon, S.S., DesHardin, P.E., Presser, C., Hewson, J.C., Avedisian, C.T., (2006), Numerical Modeling and Experimental Measurements of Water Spray Impact and Transport Over a Cylinder. *International Journal of Multiphase Flow*, **32**, 132-157.