CHAPTER 3 METHODOLOGY

In order to develop a dynamic model of polylactic (PLA) in filling stage of an injection molding process, the finite volume method, which is embedded in ANSYS CFX has to be applied in this study. The steps of this work can be divided into 4 main steps as illustrated in Figure 3.1.

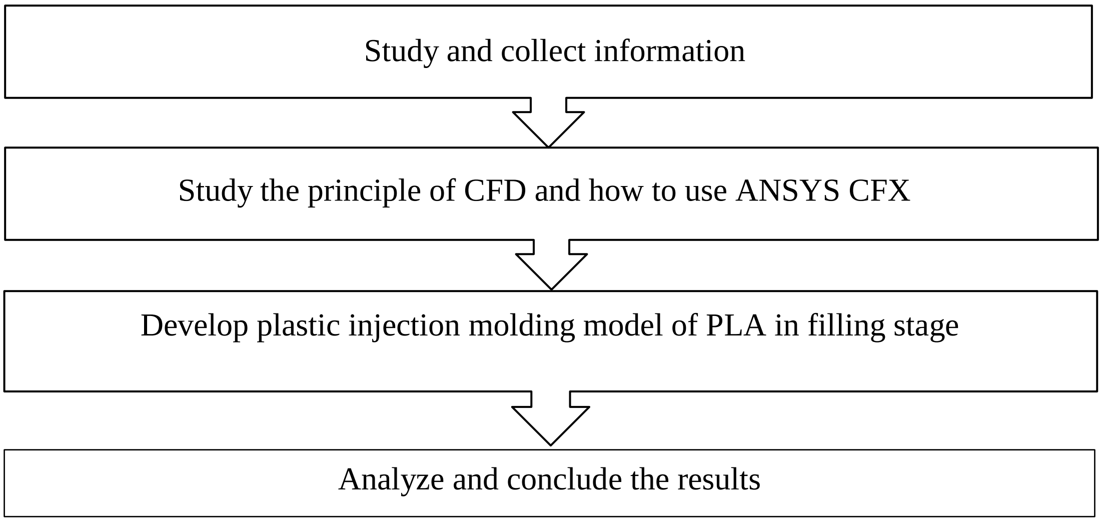


Figure 3.1 Methodology

3.1 Study and collect information

Before performing the dynamic flow behavior model of PLA in filling stage of an injection molding process, the necessary information needed to be gathered. The general principle of plastic injection molding process, the plastic injection molding parameters, the rheological properties of PLA biodegradable plastic, plastic flow characteristic and general computational fluid dynamics software, ANSYS CFX, manual and tutorials must be studied thoroughly.

3.2 Study the principle of CFD and how to use ANSYS CFX

This step mainly concentrates on the process of understanding the fundamental of computational fluid dynamics package, governing equations and its mathematical methods, which are important so as to create the dynamic flow behavior model of PLA in filling stage of an injection molding correctly.

3.3 Develop plastic injection molding of PLA in filling stage

The PLA dynamic flow behavior model is modeled in this step which can be distributed into 3 stages relating the ANSYS CFX procedure. First, the basic geometries of mold is drawn and meshed in the pre-processing stage in ANSYS CFX. The physical, fluid properties and boundary conditions must be also defined in the simulation program in order to make the simulated model more realistic. Second, the created model was solved utilizing the finite volume numerical solution technique. Finally, the simulation results were then presented in post-processing stage, respectively.

To obtain the satisfactory results from the simulation, the measured data from the actual process, e.g., machine setting, mold dimensions and material properties must be used as the inputs in simulation program which are in accordance with the boundary conditions, the mold model and the material properties. Table 3.1 is then prepared to apprehend the data connectivity between the actual process and the simulation.

Table 3.1 Data connectivity between experiment and simulation

Actual process	Simulation	Stage in ANSYS-CFX
Mold geometry	Mold model Mesh generation	Pre-processing
Fluids properties	Air properties PLA properties	
Operating conditions	Boundary condition Initial condition Model assumption	

3.3.1 Pre-processing stage

3.3.1.1 Geometry creation

The first requirement of ANSYS CFX is geometry creation based on the shape and the dimension of an actual mold as presented in Figure 3.2. This mold consists of 3 main parts which are sprue, runner (L-shape) and dog bone domains. The width and length of dog bone part are approximately 0.75 and 6.50 inches, severally. The details of mold geometry and mold dimensions are shown in Figure 3.3 and 3.4, respectively.

Figure 3.2 Actual shape of mold

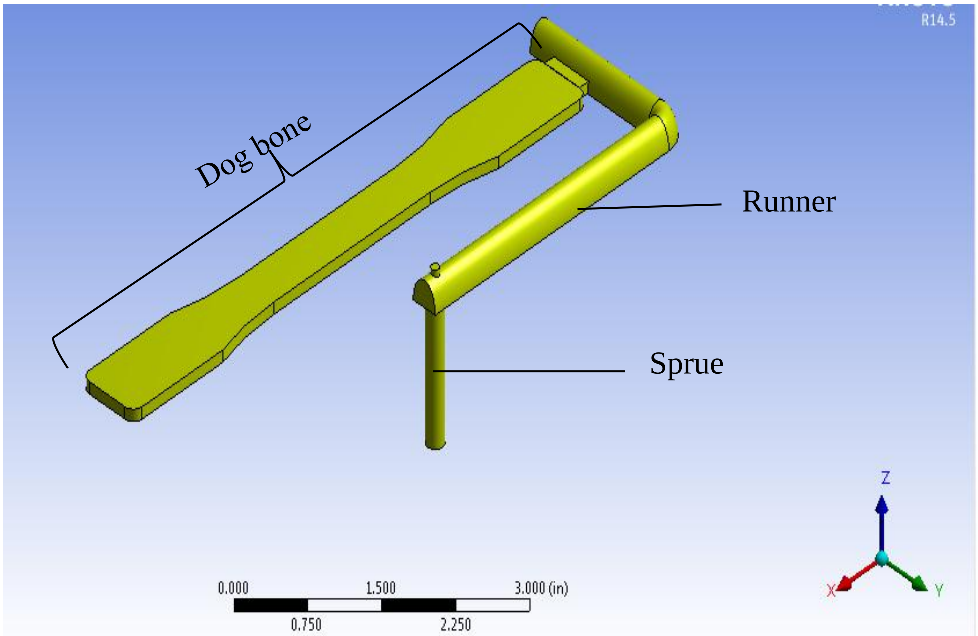
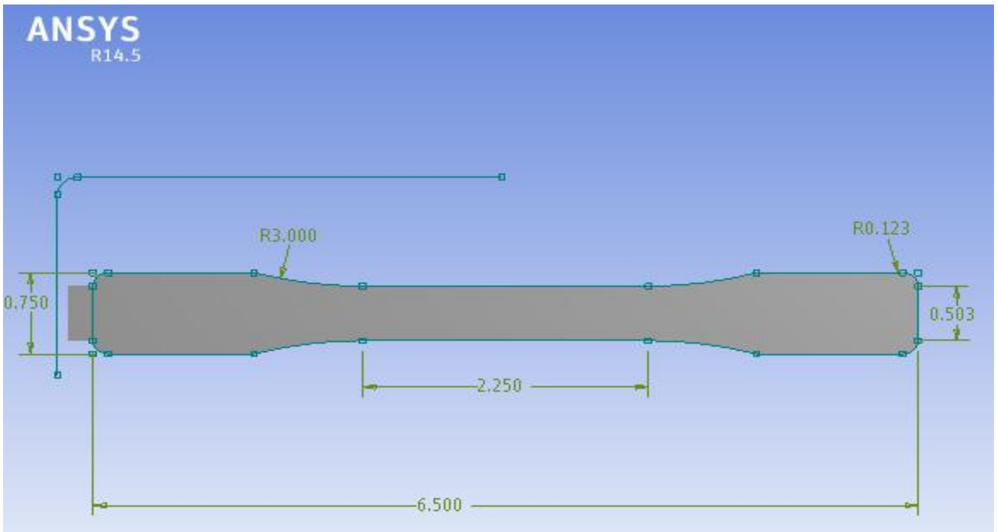
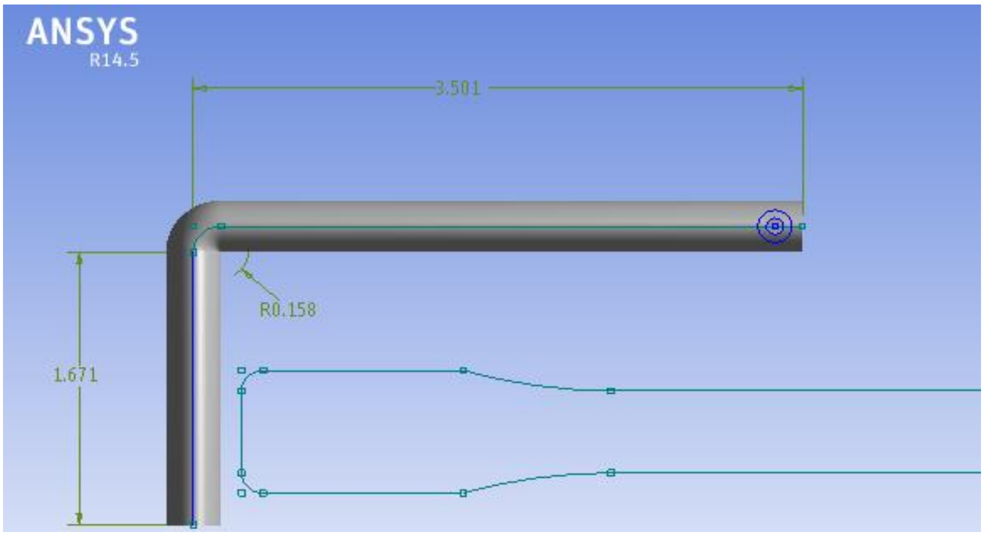


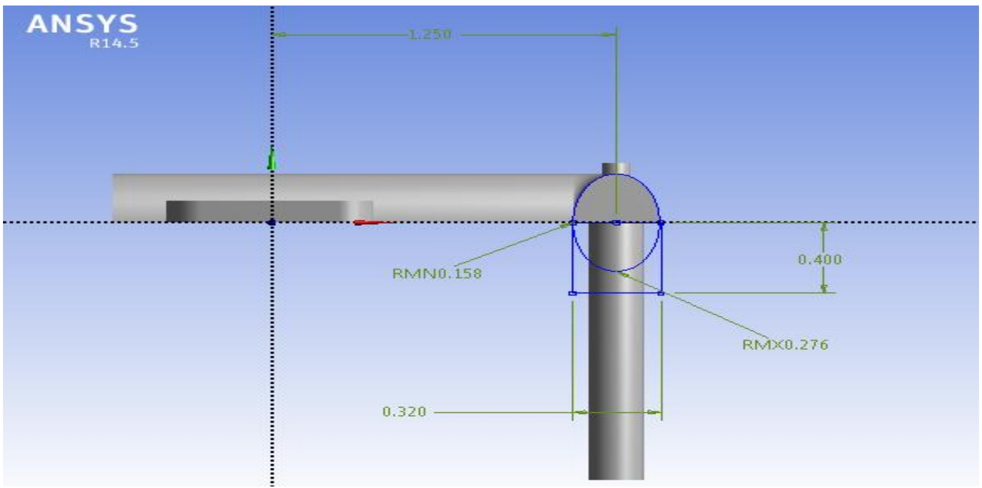
Figure 3.3 Mold model


ANSYS
R14.5
R3.000
R0.123
0.750
0.503
2.250
6.500

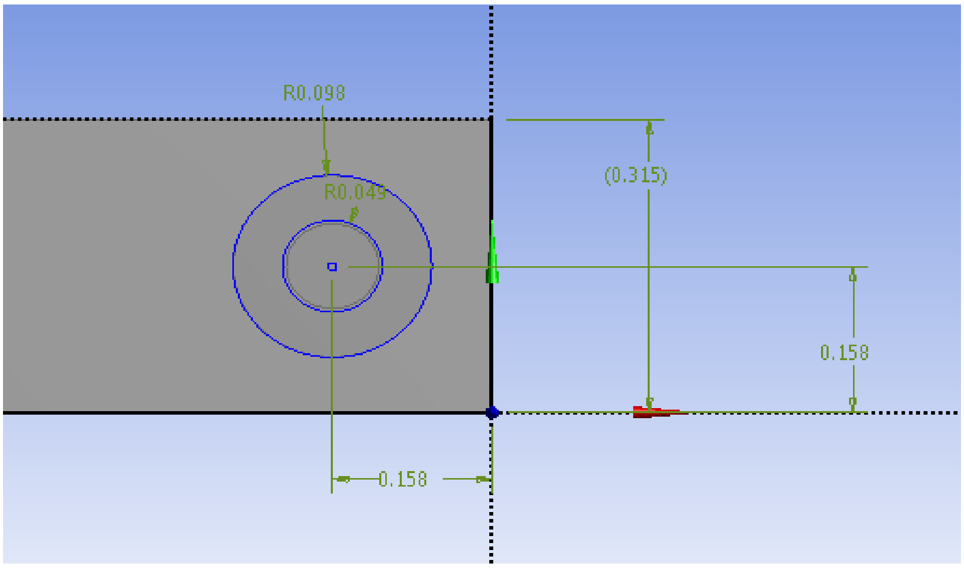
(a)


ANSYS
R14.5
3.501
R0.158
1.671

(b)


ANSYS
R14.5
1.250
RMN0.158
0.400
RMX0.276
0.320

(c)



(d)

Figure 3.4 (a) Dimension of dog bone part in inches

(b), (c) Dimension of sprue and runner parts in inches

(d) Dimension of inlet position in inches

3.3.1.2 Mesh generation

After the mold geometry was created, mesh generation was also used to detach the interested domain into smaller control volumes.

Nevertheless, to certify that the numbers of elements and nodes were large enough to resolve the governing equations correctly, the mesh independence study must be carried out by varying the numbers of elements and recording interested variable. To perform the mesh independent study, the simple fluids which are water and air was employed. In this case, the average water volume fraction was set as the monitor point value. Hence, the trend line between the average water volume fraction and the number of elements was illustrated in Figure 3.5. It revealed that even though the number of elements was refined more than 27,000 cells, the average water volume fraction was fairly stayed the same which mean that was not necessary to use the number of meshed elements over 27,000. Thereby, the mesh independent solution of model was 27,860 elements and 23,421 nodes as displayed in Figure 3.6.

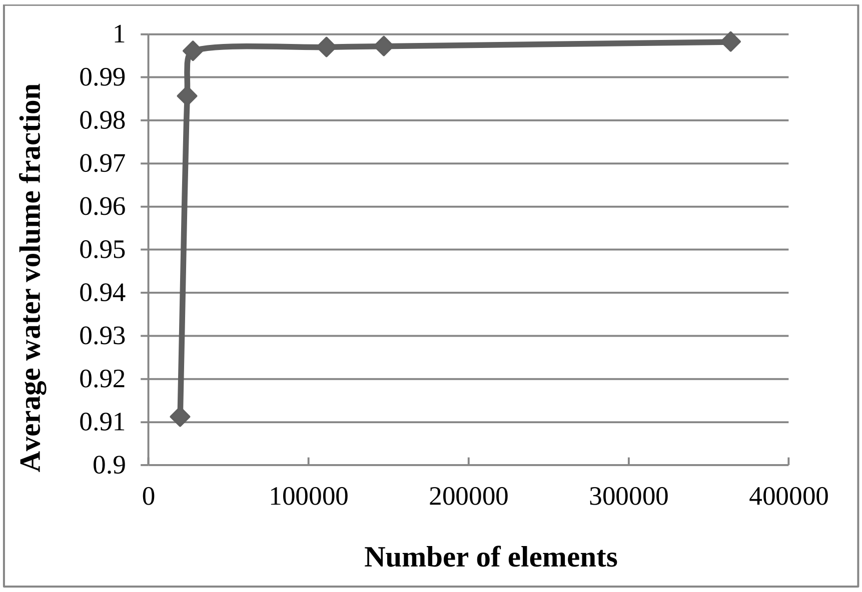


Figure 3.5 The average water volume fraction versus the number of elements

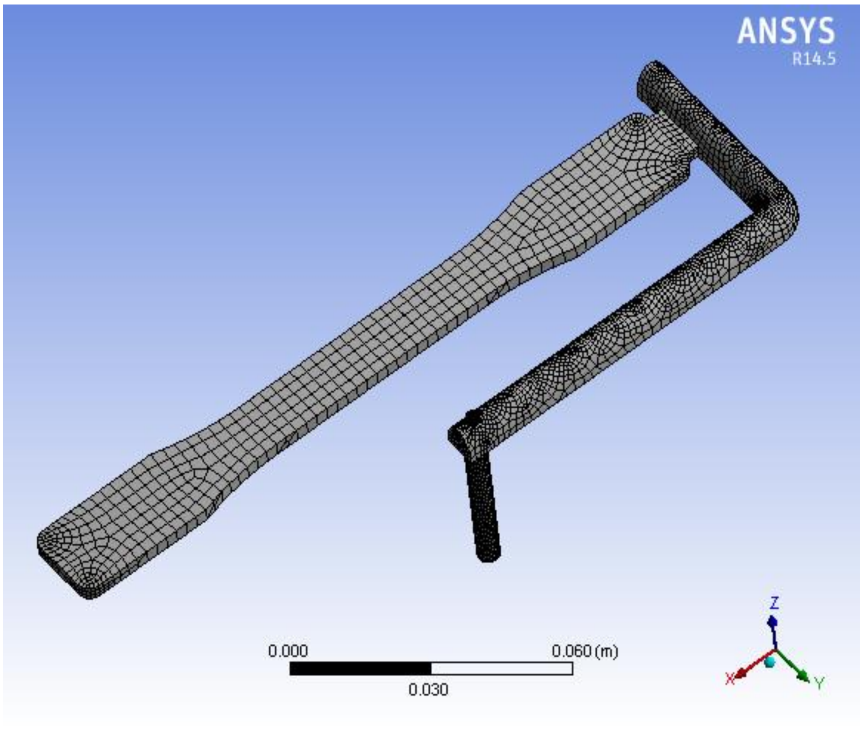
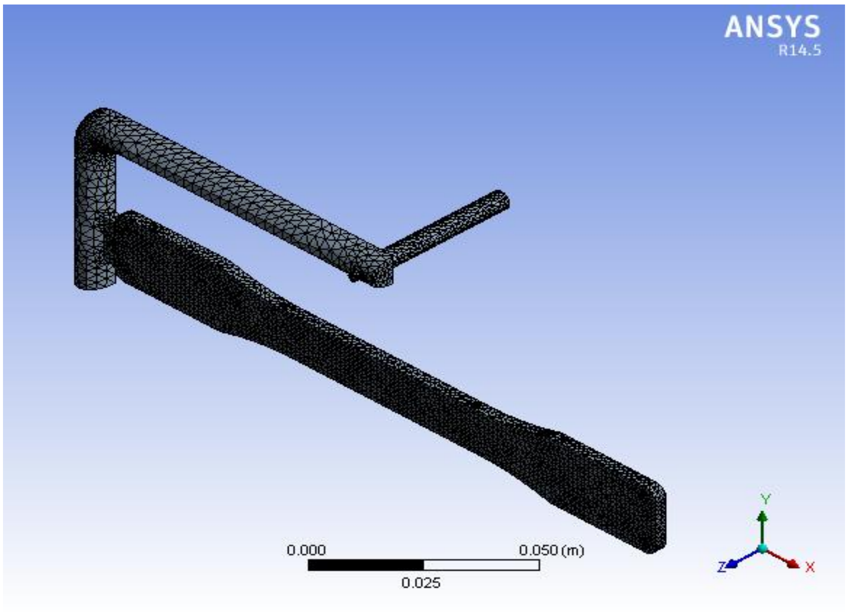
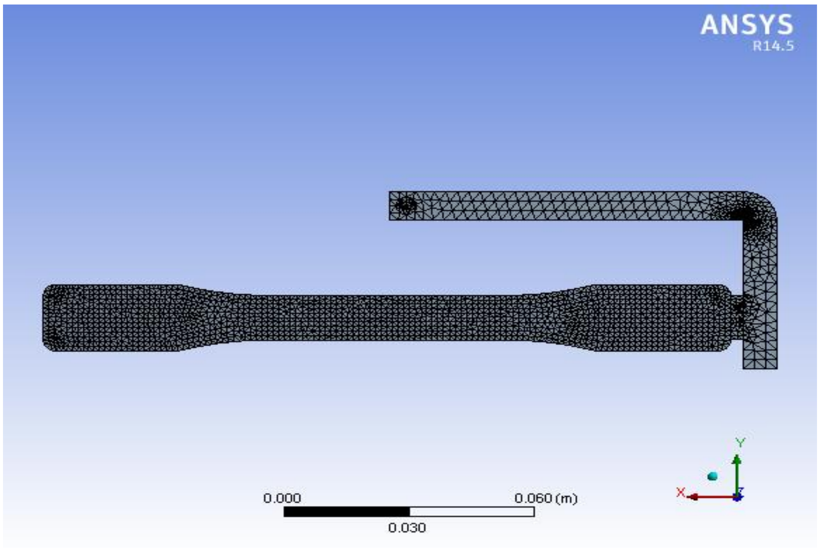


Figure 3.6 Meshed model of mold

From the Figure 3.6, the mesh elements in dog bone part seem rough more than the runner and sprue which may not be appropriate. Actually, the most important part of this mold should be the dog bone part because it is usually used as the specimen to the other plastic testing methods. This denotes that the dog bone could be detached into the finer elements than the runner and the sprue part by means of refinement function in ANSYS CFX. However, the mesh cells of runner and sprue should be kept smooth as well. Therefore, the mesh solution of model was 32,559 elements and 8,717 nodes as displayed in Figure 3.7.



(a)



(b)

Figure 3.7 (a) Meshed model of mold in xyz axis

(b) Meshed model of mold in xy plane

3.3.1.3 Selection of physics and material properties

The model used in simulation comprises of two phases of the fluids during plastic injection molding process which are air and molten PLA 7000D. The properties of air are already provided in the material database of ANSYS CFX while the material properties of PLA 7000D are reported by NatureWorks® showing in Table 3.2.

Table 3.2 Material properties of air and PLA 7000D

Material data	Air	PLA 7000D	Unit
Specific heat capacity	1,004.4	2,020	J kg^{-1} K^{-1}
Thermal conductivity	0.0261	0.195	W m^{-1} K^{-1}
Molecular weight	28.96	66,000	g mol^{-1}
Density	1.185	1,072.7	kg m^{-3}
Dynamic viscosity	1.831x10^{-5}	Cross-WLF expression	Pa.s

According to the flow of PLA in filling stage is dependent on the viscosity which is the function of melt temperature and shear rate. Hence it is necessary to use the viscosity model so as to explain the flow behavior of PLA. Cross-WLF is one of the viscosity temperature dependent viscosity relations that can be adapted to this simulation, the viscosity expression and its data fitted coefficients of Cross-WLF model are written in terms of CFX Expression Language (CEL).

3.3.1.4 Specification of boundary and initial conditions

In order to create the PLA flow behavior in filling stage model more practical, the model assumptions, the boundary and the initial conditions must be completely specified in simulation program. However, the specification only initial and boundary conditions are not enough to treat the simulation more realistic so the reasonable model assumptions of this fluid flow problem were additionally set as follows;

1) Laminar flow
2) Transient condition
3) Non-isothermal system
4) Non-Newtonian fluid
5) Incompressible fluid
6) Inhomogeneous and two phases flow
7) No phase changing or solidifying

To set the boundary and initial conditions of mold filling analysis in ANSYS CFX, the actual operating conditions of plastic injection molding process were collected by comparing to different melt temperatures of 175, 190 and 230°C which are in accordance with the recommended melt temperature range of 170-230°C [8]. The operating conditions are provided in Table 3.3

Table 3.3 The operating condition of plastic injection molding process

Process conditions			
Injection velocity (m/s)	0.382	0.382	0.382
Injection time (s)	5	5	5
Injection temperature, T_{melt} (°C)	175	190	230
Mold temperature, T_{wall}(°C)	30	30	30

So as to specify the initial and boundary conditions reasonably, the details on filling stage in plastic injection molding process could be explained. Initially, the mold cavity is assumed to be rest and full of air and the molten PLA is being pushed the air the cavity out of mold during injection molding.

Therefore, the initial conditions over the domain are fluids at rest, pressure equal to zero, temperature of air and PLA are 30°C based on a constant mold temperature. Owing to mold model is filled with air hence the initial air and molten PLA volume fractions are 1 and 0, severally. The details of the initial conditions are expressed below.

At t=0;

Velocity = 0

Relative P = 0

T_{air}=T_{PLA}=T_{wall} = 30°C

Volume fraction : air=1, PLA=0

In addition, the outlet or air vent was designed to allow only air to go through mold cavity while the inlet only allows molten PLA to flow into cavity. The positions of inlet, outlet and mold wall are displayed in Figure 3.8.

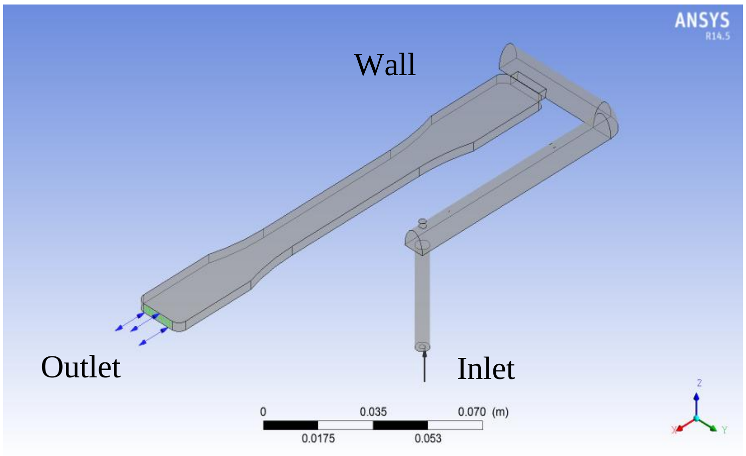


Figure 3.8 Position of inlet, outlet and wall of mold model

For boundary conditions, the injection velocity of molten PLA of 0.382 m/s was used in model together with 5 seconds of filling time and specified melt temperature. The buoyancy model is also regarded by specifying the reference density of air, 1.185 kg/m^3, and setting buoyancy gravity y=g based on the mold geometry. The boundary conditions are summarized below:

On mold wall: $u = v = w = 0$; $T = T_{wall}$

At inlet : $T = T_{melt}$

At outlet : $P_{outlet} = 0$

After the pre-processing stage was already done, the processing stage will be employed in order to numerically solve the governing equations by way of the high resolution advection scheme. The time step size is indicated to 10^{-4} seconds together with maximum number of coefficient loops of 2,000. Besides, 10^{-3} is set as the convergence criteria based on the RMS residual type and the Second Order Backward Euler is provided as the transient scheme of the solver control in simulation, respectively.

3.4 Analyze and conclude the results

The simulation model of plastic injection molding and the accurate results from previous step are then used to analyze and conclude. The effects of melt temperature on viscosity, and shear rate are also plotted and studied. The flow behavior of PLA in injection molding from ANSYS CFX is interpreted in this section. Furthermore, the effect of important parameters, melt temperature and filling time, which influence on the PLA plastic product are discussed as well.