CHAPTER IV

COMPUTATIONAL FLUID DYNAMICS (CFD): MODEL SETUP

Currently, the CFD technique is widely used in many applications. Engineers and researchers use CFD to design, analyze, and simulate fluid flows in interested devices such as turbo machinery, wind tunnels, and aerodynamics applications. Although, there are numbers of ready commercial CFD software and codes being available for use, in order to obtain good results and analysis in fluid dynamics problems good knowledge in the physics of the problem and basic understanding of numerical methods is required. Moreover, validation of the CFD results with real experiments should also be performed so that the results are creditable.

For this study, the finite volume method in a commercial CFD package (FLUENT 6.0) is used to simulate the flow and predict the performance of the R141b ejector. This chapter provides the informative description of the theory and assumptions used for the simulation. Basic information on setting up the calculated model and the mesh generation method are also presented.

4.1 Introduction to Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics is a branch of fluid mechanics employing numerical methods and algorithms to solve and analyze the systems involving fluid flows. If the problems or systems are complex, computers may be required in order to compute a numerical solution. Generally, the algorithm of the CFD is composed of pre-processing step, solver step and post-processing step. Pre-Processing is a process that uses a post-processor in identifying the system geometry (physical boundaries) and the system volume inside the physical boundaries is divided into a number of discrete cells (mesh). All necessary information on fluid properties at the boundaries is defined. The simulation step (Solver Step) is the step of solving all equations of a specified problem numerically and iteratively. Fluid Dynamics problems always involve numbers of partial derivative equations of the Navier-Stokes equation in the conservative form of energy, mass and momentum. Some of the discretization methods being used for solving those equations are finite volume method (FVM), finite element method (FEM) and finite difference method. Finite Volume Method, the classical and the most used in commercial CFD codes, employs the control-volume-based technique to convert all governing equations into an algebraic form that can be solved numerically. This control volume technique consists of integrating the governing equations about each control volume, yielding discrete equations that conserve each quantity on a control-volume basis. Post-Processing is a process in which a post-processor program is used to view, present, and analyzes the results. The resulting solution can be plotted and presented graphically.

As mentioned previously, fluid dynamics problems might be complex and the partial derivative equations could be composed of many terms. Hence the finite volume method for commercial CFD codes needs good algorithms of equation solving steps. Basically, there are 2 solution methods, the segregated and the coupled solver. The segregated solver is the solution algorithm in which, the governing equations are solved sequentially. Several iterations of the sequential solution are continued until the convergence criteria are satisfied. Whereas, the coupled solver performs its solving step by solving the governing equations of mass, momentum, and energy simultaneously (i.e., coupled together). To reach a converged solution, several iterations of the coupled solutions must be performed.

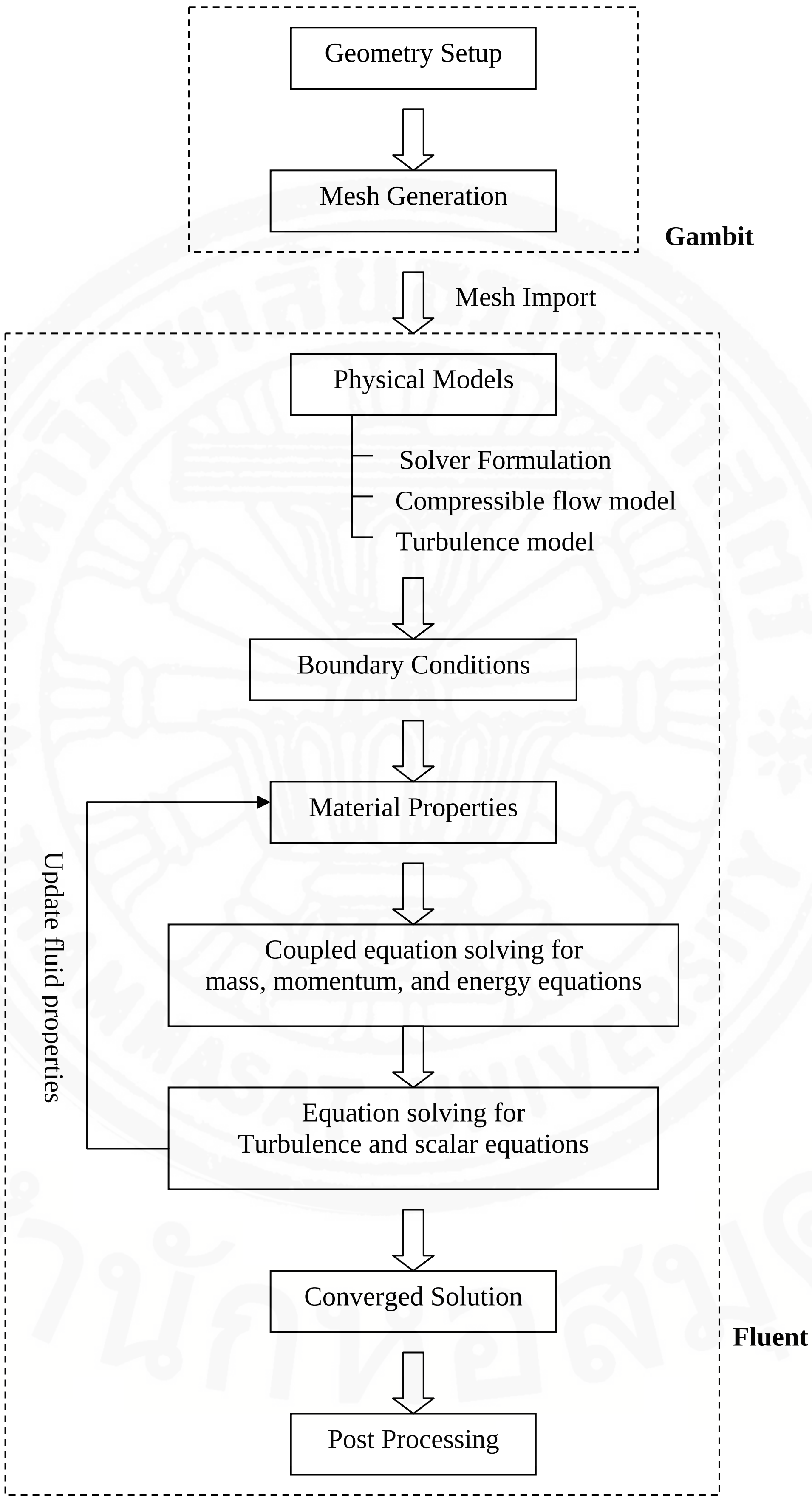


Figure 4.1 Flow chart of the CFD procedure for modeling the R141b ejector.

4.2 CFD Technical Data for the Current Study

The problem under investigation here involved the supersonic flow inside the flow passage of the experimental R141b ejector. Working conditions of the model were set at the same ranges as was done in the experiments. In order to simulate this particular situation, Gambit 2.1 and FLUENT 6.0 were used as the pre-processor to generate grid network (mesh) and the CFD solver, respectively. The procedure of using the Gambit 2.1 and FLUENT 6.0 for this analysis is shown in Figure 4.1.

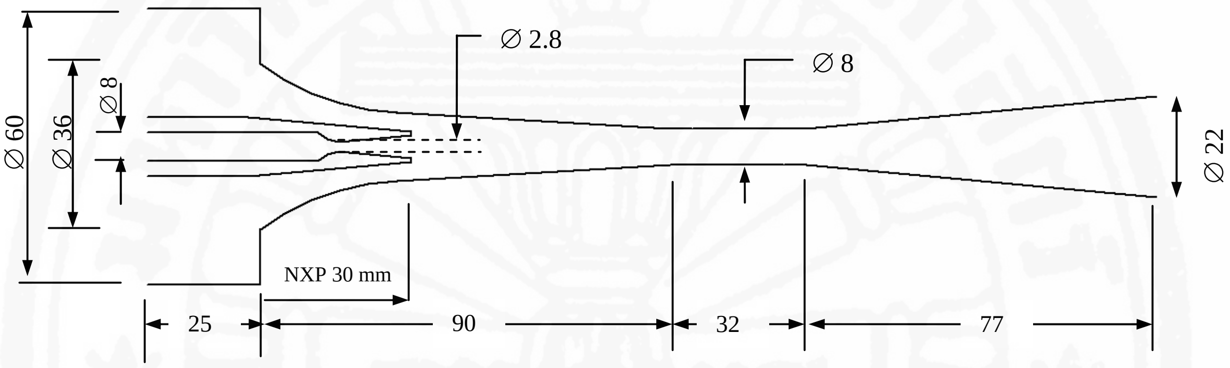
4.2.1 Modeling Assumptions

These following assumptions are made in order to perform the CFD analysis for an ejector:

- The flow is assumed to be steady and two-dimensional compressible flow.
- The flows at all inlets are accelerated from their stagnation points.
- The flow is turbulence.
- The property of working fluid is set as an ideal gas.
- Wall boundary condition of the ejector was set as adiabatic wall and was assumed to be stationary and non-slipped surface.

4.2.2 Geometry setup

As proposed, Gambit version 2.1 was used as a preprocessor to create the calculation domain of the models. The geometries of the calculation domain of the modeled ejectors were taken from those which were used in the experiment. For example, Figure 4.2 a) presents an ejector model that used primary nozzle No.1, throat No.1 and mixing chamber No.1. Their significant dimensions have already been described in Chapter 3. The models were created in a two dimension (2-D) domain. The 2-D domains of the ejector were created in a rectangular coordinate x-y. Since, in the Fluent step, the axisymmetric model was applied to the simulation, the geometry was dimensioned only above the x-axis as shown in Figure 4.2 b). The two-dimensional axisymmetric model had axial symmetrical domain about the x-axis. The advantage of using the two-dimensional axisymmetric model was that the three-dimensional effect (3-D) was taken into account in the simulation.



a) Full shape of the geometry with dimensions (Units in millimeters).

b) Axisymmetric geometry in Gambit 2.1.

Figure 4.2 Geometry setup for the R141b ejector.

4.2.3 Meshing the model

The grid network models were meshed using a mesh function in Gambit 2.1 and then were transferred to FLUENT. Grid structures of the models were meshed using the normal quadrilateral grid. Since concentration of the grid density is critical to the stability and the convergence of the simulation, the grid network models were focused and dense on the areas where the large gradient in fluid properties and the significant flow phenomena were expected. For example, the grid was dense at the place where the primary fluid and the secondary fluid were mixed and where the shock phenomenon was likely to occur. In the nature of the flow through an ejector where shock and turbulence are common, the near wall boundary layer needs to be meshed at the boundary layer. Grid structure for the 2-dimensional ejector model corresponding to the geometry model in Figure 4.2 is shown in Figure 4.3. The mesh was made of 43,000 structured quadrilateral elements. To investigate the effects of geometry on the flow of the R141b ejector, the number of grid elements was changed when the computational models were changed corresponding to the change in geometrical experimental investigation. To ensure the stability of the simulated solutions with grid independence, a grid refinement (increasing grid numbers to around 80,000) was performed. After refining the grid elements, the solutions of the models with the order of 40,000 elements and 80,000 elements were found no different. Thus, considering the mesh resolutions, the numbers of grid elements of all models were set high enough (in the order of 40,000 elements) to capture all the flow features inside the ejector.

4.2.4 Solver Formulation

FLUENT [51] provides three optional solver formulations: segregated, coupled-implicit, and coupled-explicit. Before any case of the simulation could be performed, one of the solver formulations should be assigned to the calculation model. The segregated solver is the default solver set in FLUENT. It can be applied to many practical flows. However, the solver used in this study was selected as a coupled-implicit solution. This solver is suitable for a case of high speed compressible flow. In the calculation process, the coupled-implicit solver couples the flow and energy equations; hence, the faster converging solution results. The disadvantage of using the couple solver is that it requires about 2 times the memory resources of the segregated solver. The couple-explicit solver may be considered if less memory is required. However, it consumes more computational time to reach a converged solution.

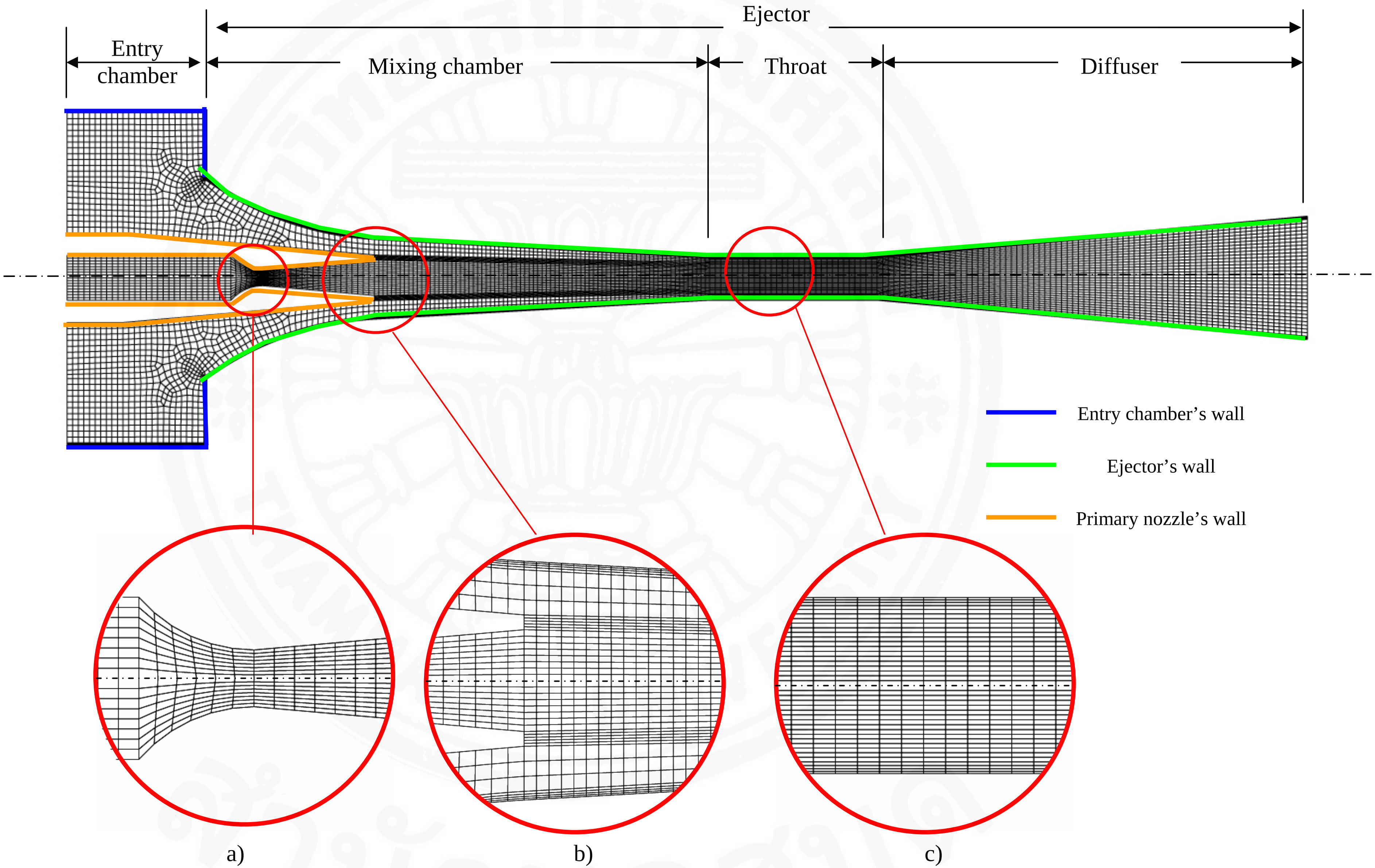


Figure 4.3 Calculation domain and grid structure of the R141b ejector CFD model.

4.2.5 Compressible Flows Model

Compressible flows can be classified by the flow velocity of a gas (U) over the speed of sound in the gas (C), which are combined to a single parameter called Mach number, M.

$$M = \frac{U}{C} \tag{4.1}$$

Since compressibility effects become important for transonic flow and supersonic flow, the compressible flows model should be applied to the calculation. Especially for supersonic flow, the flow may contain shocks and expansion fans which can impact the flow pattern significantly.

In FLUENT, it is not necessary to set up any special cases to handle the compressible flow assumptions. FLUENT solves the continuity and momentum equations by incorporating the flow speed and its related static pressures and temperature given in the boundary setup procedure.

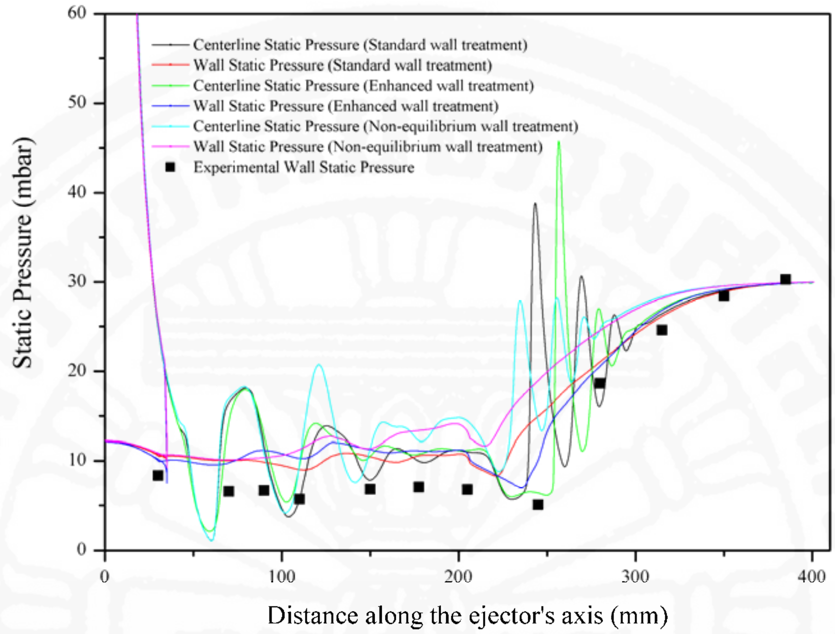
4.2.6 Turbulence model

Due to the high speed flow in the ejector channel, the flow model is set as realizable k-epsilon model which is one of the turbulence models provided in FLUENT. The realizable k-epsilon model satisfies certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows in which both the standard k-epsilon model and the RNG k-epsilon model are not applicable. For the case of the flow in ejectors, the realizable k-epsilon model provides the spreading rate of round jets more accurately and suitably for flows under strong adverse pressure gradients as expected to occur for the flow in ejectors.

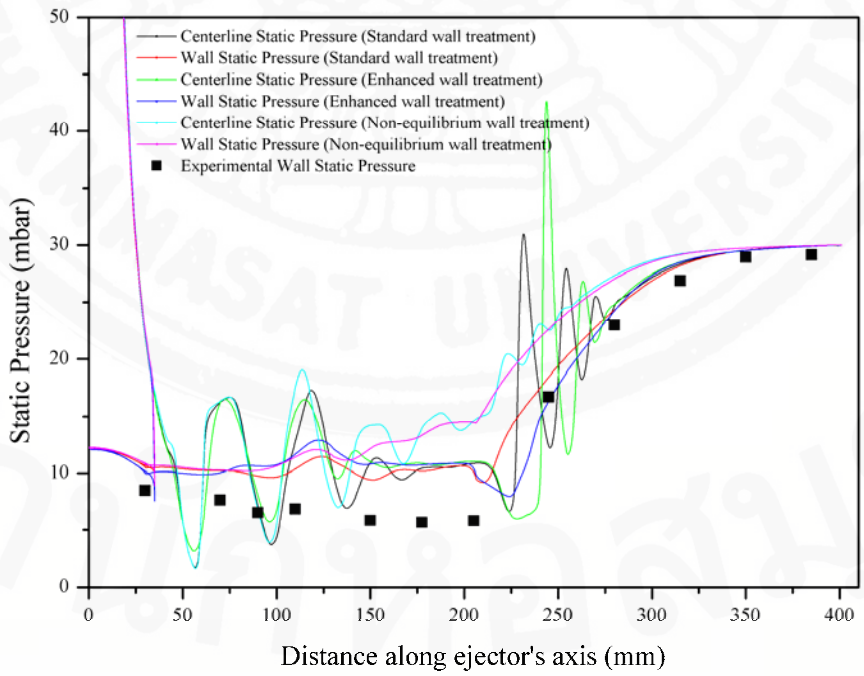
4.2.7 Wall functions

Turbulent flow behaviors at the region close to the wall are always exclusive to the CFD solver. Accurate representation of the flow in the near-wall region determines successful predictions of wall-bounded turbulent flows. Two different near-wall flow representations or wall functions are provided in FLUENT [51], standard wall function and non-equilibrium wall function. The standard wall function gives reasonably accurate predictions for the majority of high-Reynolds-number, wall-bounded flow. The non-equilibrium wall function further extends the applicability of the wall function approach by including the effects of pressure gradient and strong non-equilibrium. However, the wall function approach becomes less reliable when the flow conditions depart too much from the ideal conditions underlying the wall function, for example, a low Reynolds number flow, boundary layer separation flows, buoyancy-driven flows. In such cases, the enhanced wall treatment provided in FLUENT is required to account for accurate mesh resolution and the near wall modeling approach.

To ensure the completeness of the standard wall treatment to the successful results of the R141b ejector, previous results from the study of Chunnanond [47] were manipulated to account for the effect of three different near-wall approaches. As seen from Figure 4.4, the results of static pressure distributions obtained from the model using the non-equilibrium wall function provided the worst agreement with the experimental values. The CFD's result using the enhanced wall treatment assumption provides the closest results of static pressure in the diffuser region compared to the experimental values. However, using the enhanced wall treatment approach consumes much more computational time than others. Even though, the standard wall function provides a larger error in calculated pressure in the diffuser part compared to the enhanced wall treatment, upstream of the diffuser the results are similar to those obtained using the enhanced wall function. Moreover, the standard wall treatment consumes much less computational time compared to the other wall approaches.



a) At T_P = 130 °C, T_S = 10 °C and P_b = 30 mbar.



b) At T_P = 120 °C, T_S = 10 °C and P_b = 30 mbar.

Figure 4.4 Static pressure profiles for different wall treatment assumptions for a steam ejector (manipulated from data provided by Chunnanond [47]).

It was also reported by Sriveerakul et al. [39~40] that the simulation results of a steam ejector using the standard wall function provide accurate results compared to the experimental values. Therefore, in this study, the standard wall function was selected to use in setting up the simulated models.

4.2.8 Boundary conditions

By ignoring the heat transfer in the calculation, the wall was simply set to be non-conducting (adiabatic) wall. Pressure inlet and pressure outlet conditions were applied to the entrances and exit of the models. Two pressure inlet conditions were set for the primary fluid inlet (the vapour-generator saturated condition) and the secondary fluid inlet (the evaporator saturated condition). A pressure outlet boundary condition was set for the discharge of the ejector (the condenser condition).These conditions were varied with the same ranges as were conducted in the experiments. The values of each boundary were assigned as the saturation properties (temperature and pressure) of each operating state. Since the velocity of the flow entering and leaving the domain was thought to be relatively small compared with the supersonic speed during the flow process of the ejector, there was no difference between an input of the stagnation pressure and static pressure.

In fact, the arrangement of the ejector in the system could be either in horizontal or vertical setting, with no significant difference from each other due to a very high speed fluid flow in the flow channel. However, if heat transfer needs to be considered, the difference in horizontal and vertical flow may not be neglected.

4.2.9 Working fluid properties

The working fluid properties of the R141b in the models were treated using the assumption of an ideal gas. Even though the ideal gas relation seemed to be an unrealistic assumption to the model, for ejector applications where the operating pressure is relatively low, it was proved by some researchers [26] that it provided similar results to a real gas model. The properties of R141b vapour, as provided in FLUENT database, are shown in Table 4.1. Note that, the density of the working fluid is evaluated using the ideal gas relation as part of the calculation as it progresses. Other properties are defined as constant throughout the simulation.

Table 4.1 Fluid properties of selected refrigerant R141b.

Property	Physical property data
	R141b
Replaces	R11
Chemical formula	$CCl_2F\text{-}CH_3$
Molecular weight	117.0
Boiling point at 1 atm (°C)	32.05
Liquid density at 25°C (kg/m^3)	1234

For a compressible flow, the ideal gas law is expressed in the following equation.

$$\rho = \frac{P_{op} + P}{RT} \tag{4.1}$$

Where P is the local relative (or gauge) pressure predicted by FLUENT and P_{op} is defined as the operating pressure which was absolute zero for this study.

4.3 Convergence Criteria

The CFD simulation of the ejector model was considered as converged and its data was ready to be proceeded when the following 2 converging criteria were satisfied. Firstly, it had to be shown that the calculated mass fluxes of every face in the model were stable. In addition, to conserve the mass, the summation of mass fluxes that entered the domain should be equal to that which left the domain. Secondly, every type of the calculation residual must be reduced lower than the specified value (in this case, less than 10^{-6}).

4.4 Results

After the CFD solution of each simulation was considered as converged, three significant types of the solution data could be presented which were:

- The entrainment ratio of the ejector
- The X-Y plot of static pressure distribution along the ejector wall and along the centerline of the ejector
- The contours of Mach number inside the ejector

The entrainment ratio (Rm) of the ejector by this simulation approach is simply evaluated from the ratio of the sum of mass flux entering the mixing chamber inlet's face to the sum of mass flux entering the primary nozzle inlet's face, both of which can be directly determined in FLUENT.

Please note that the simulated entrainment ratio and the static pressure profile along the ejector wall were the 2 most significant parameters in validating the CFD results with the experimental results. If the comparison showed the similarity between the results from both approaches, then the correctness of the simulated CFD model was verified. Thus, other related solution data obtained from the CFD, such as the static pressure profile along the centerline of the ejector and the contours of Mach number or the plot of the Mach number could be fairly used to explain and represent the flow inside the ejector.

4.5 Conclusions

In this chapter, the background of the CFD technique was presented. The criteria of creating the calculation domain, grid elements, and the information of the CFD ejector model setup (fluid properties, solver selection, turbulence model and boundaries conditions), including the convergence criteria and types of solution data to be considered were provided and summarized as shown in Table 4.2.

Before the analyses of the simulated results were made, some of them had to be validated through the reliable data from the experiments. In the next chapter, the validation process of the simulated results with the experiment results measured from the constructed R141b ejector refrigerator is presented. After the correctness of the model was guaranteed, then other calculated information obtained from the CFD models could be used to represent the flow phenomena and the mixing behaviors in the R141b ejector, as will be discussed in Chapter VI, VII and VIII.

Table 4.2 Setup information of the CFD model.

Criteria of numerical model	Selected criteria
1. Domain	Axisymmetric domain
2. Boundary conditions	
Inlet boundary condition	Pressure inlet condition
Outlet boundary condition	Pressure outlet condition
3. Meshing information	43,000 structured quadrilateral elements
4. Solver formulation	Coupled-implicit solution
5. Turbulence model	Realizable k-epsilon model
6. Working fluid	R141b (CCl_2F-CH_3)
7. Wall-treatment method	Standard wall function
8. Convergence criteria	Calculation residual less than 10^{-6}