

CHAPTER 4

COMPUTATIONAL FLUID DYNAMICS (CFD): MODEL SETUP

In this Chapter, the introduction of computational fluid dynamics CFD technique is introduced. The details of creating physical model and solver setup are explained. In the part of creating physical model, the commercial software package, Gambit 2.3 is used. The mathematical model suitable with flow inside the ejector is provided by commercial software package, FLUENT 6.3.

4.1 Introduction to computational fluid dynamics

The computational fluid dynamics (CFD) technique employs the principle of numerical method to transform governing equations of the flow to be algebraic form so that it can be solved numerically. In fluid dynamics problem, the governing equation is mostly written in terms of partial derivative equation of Navier-stokes equation in the conservative form of energy, mass and momentum.

There are three methods in order to transform all governing equation, the finite difference method (FDM), the finite element method (FEM) and the finite volume method (FVM). The most widely used method in order to transform all governing equation to algebraic form is the finite volume method (FVM). This method discretises the governing equation by first dividing the physical space into number of arbitrary polyhedral control volume (grid elements). The surface integral is approximated by the sum of fluxes crossing the individual faces of the control volume. Therefore, it can be seen that the physical model of fluid dynamics problem is necessary divided as the grid elements so that it can be solved numerically.

Normally, the algorithm of using the CFD technique is composed of pre-processing step, solver step and post-processing step. Some details for each of steps are presented as follow:

4.1.1 Pre-processing step

Pre-processing step is a process that uses a pre-processor in identifying the system geometry (physical boundaries). The system volume inside the physical boundaries is divided into a number of discrete cells (grid element). Generally, this pre-processing step consists of the input of a flow problem by means of an operator-friendly interface and the subsequent transformation of this input into a form suitable for use by the solver. The activities of the pre-processing step involve:

- Definition of the geometry of the region interest: the computation domain
- Grid generation of the domain into a number of smaller elements (grid elements).
- Selection of the physical and chemical phenomena that need to be modeled.
- Definition of fluid properties.
- Specification of appropriate boundary conditions at cells which coincide with or touch the domain boundary.

4.1.2 Solver step or simulation

The solver step (simulation) is the step of solving all equation of a specified problem numerically and iteratively. The numerical algorithm consists of the following step:

- Formal integration of the governing equation of the fluid flow over all the (finite) control volumes of the solution domain.
- Discretises involves the substitution of the variety of finite-difference-type approximations for the terms in the integrated equation representing flow processes such as convection, diffusion and sources. This converts the integral equations into a system of algebraic equation.
- Solution of the algebraic equations by an iterative method.

4.1.3 Post-processing

This post-processing step is the step that presents the results obtained from the solving step. Thus, these results are easy to analyze. This post-processing step involves:

- Domain geometry and grid display
- Vector plots
- Line and shaded contour plots

- 2D and 3D surface plots
- Particle tracking
- View manipulation (translation, rotation, scaling etc.)
- Color postscript output

In order to achieve the realistic flow of fluid, the partial derivative equation may be combined by many terms of mathematical model. Thus, the fluid dynamics problem may be more difficult. To solve this problem, the computer program may be required. Therefore, currently, many commercial CFD software packages are created to support the user.

4.2 CFD technique: Application in steam ejector

It is well known that the flow inside the steam ejector can be considered as a fluid dynamics problem. Thus, the CFD technique can be used to simulate the flow inside the steam ejector and predict its performance. In this study, the CFD technique is used to predict the steam ejector's performance and to simulate the flow inside the steam ejector. In the case of pre-processing step (creating physical model), a commercial software package, Gambit 2.3 is used to create the physical model and grid elements. Meanwhile, solver and Post-processing step, a commercial software package, FLUENT 6.3 is used to simulate and analyze the flow behavior inside the steam ejector. The flow chart of the CFD procedure is presented in the figure 4.1



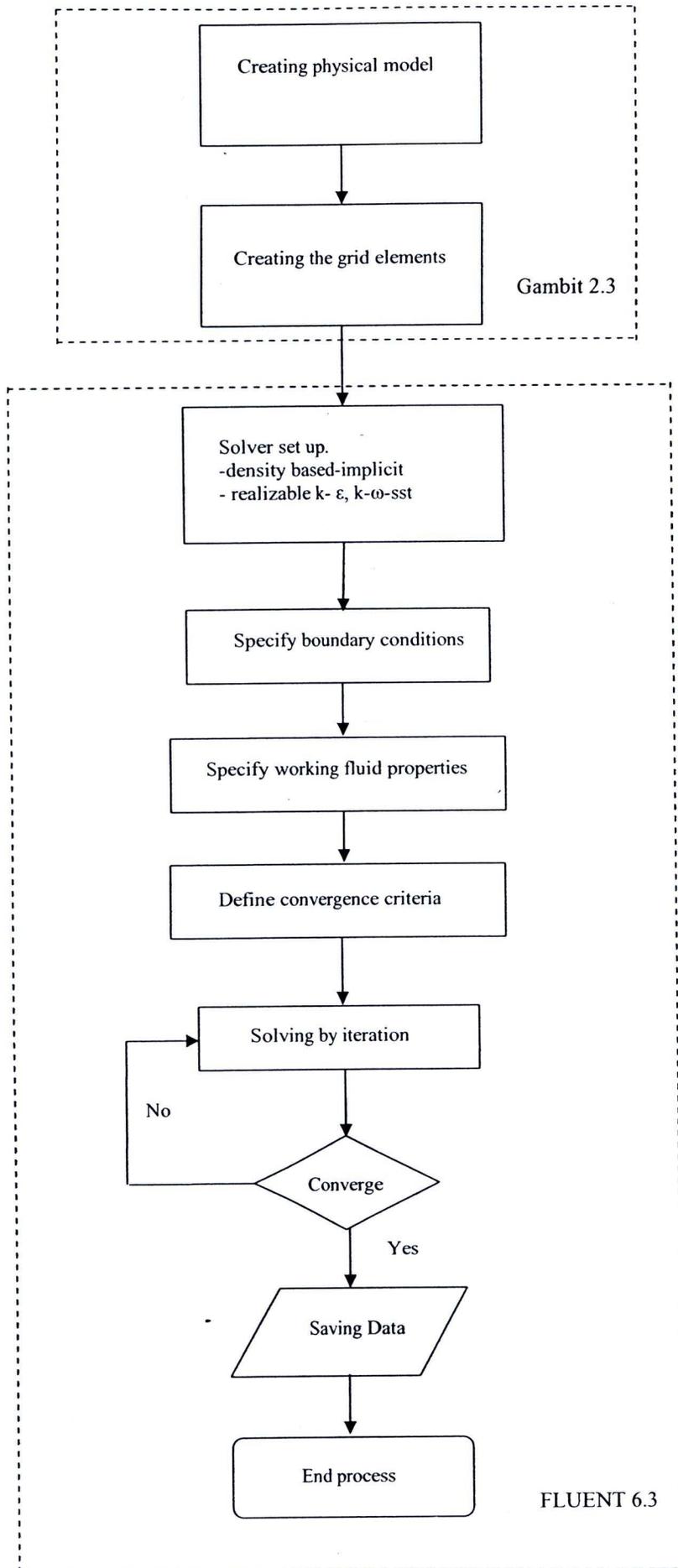


Figure 4.1: The flow chart of the CFD technique

4.2.1 Assumption of CFD modeling

Normally, to analyze the fluid dynamics problem, all necessary assumptions must be provided. The assumptions of the CFD model are provided as follow;

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

4.2.2 Creating physical model

In this case, the geometries of physical model's steam ejector were created as the same dimension as the experimental steam ejector by using the commercial software, Gambit 2.3. Consider to this problem (flow inside the ejector), the three dimensional (3-D) effect should be suitable with this case. However, the 3-D model required very long time for calculation. From the literature available [27], it was shown that the *two dimensional-axisymmetric model (2-D axisymmetric model)* provided the simulated result to be similar to that obtained from the 3-D model. Meanwhile, it required less time for calculation than that of the 3-D model. Therefore, in this study, the *2-D axisymmetric model* was applied to investigate the steam ejector performance. The *2-D axisymmetric model* had axial symmetrical domain about the x-axis.

This physical model was divided as grid elements by mesh function in Gambit. The grid elements were created in the form of equilateral elements. During the investigation, the grid elements were created of 44,000 elements as shown in figure 4.2. The grid network model was focused on the area where the significant flow phenomena were expected to occur. In this case, the grid was dense at the area where the mixing process and the shock phenomenon are expected to occur. In addition, the near wall boundary layer was also created so that the flow closer the ejector's wall was more realistic. However, the concentration of the grid elements is directly related to the stability and the convergence of the solution. To ensure that the solution was independent of grid structure, during the simulation, the grid refinement (increasing grid elements to around 80,000) was performed.

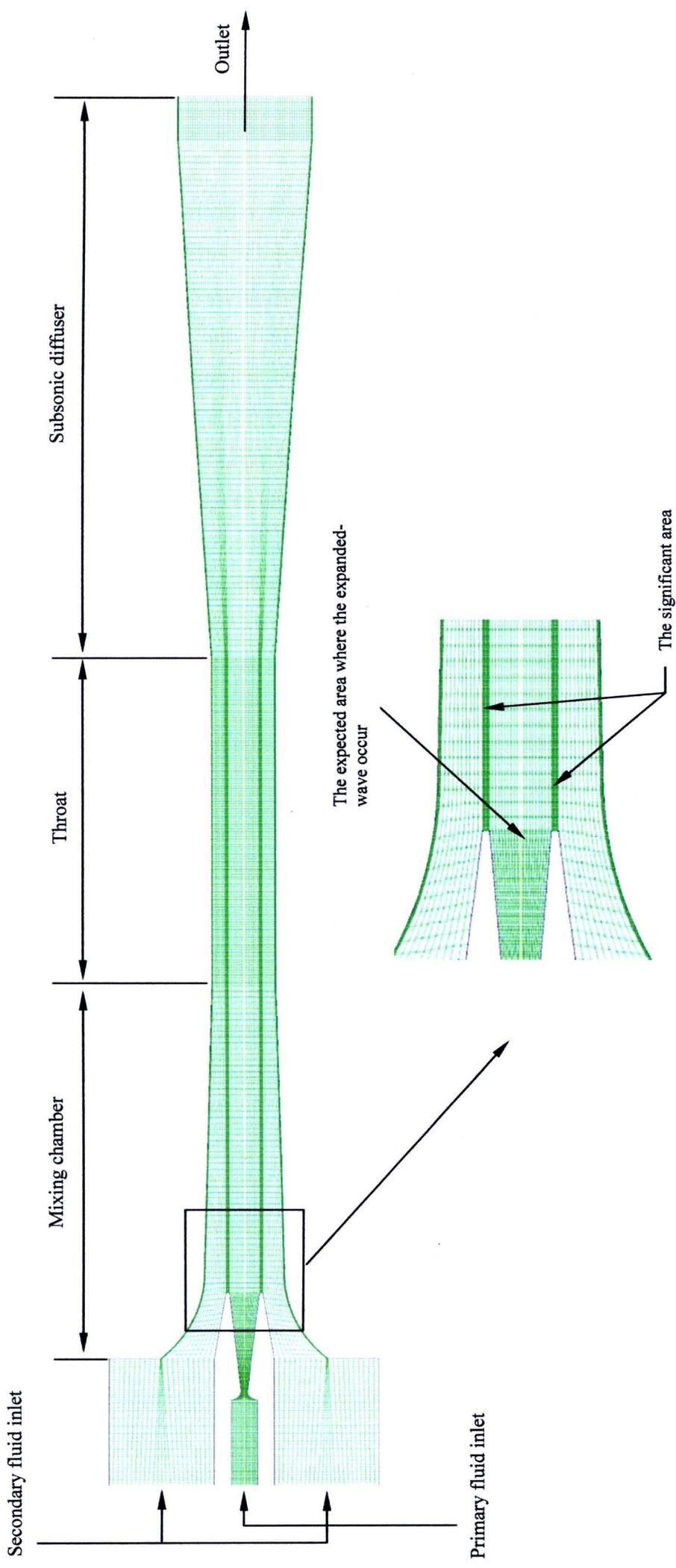


Figure 4.2: The physical model and grid structure of the ejector.

4.2.3 Solver setup

In this study, the CFD commercial software package, FLUENT 6.3 was used to apply the mathematical model for the physical model as proposed above. Consider to the flow inside the steam ejector; a turbulence compressible flow model was applied. In FLUENT 6.3, it provides three optional solver formulations suitable with supersonic flow field, *pressure-based implicit*, *density-based implicit* and *density-based explicit*. In this study, the *density-based implicit* was selected as a solver. This solver is suitable to the case of high speed compressible flow [3, 4, and 16]. During the calculation process, this solver couples the flow and energy equation. Thus, the faster convergence of solution is the result. However, the major disadvantage of using the density based implicit solver is that it requires about 2 times the memory resources of the other solvers.

The *density-based implicit* solver was combined with a turbulence viscosity model so that the flow inside the ejector is more realistic. In this case, the *realizable $k-\epsilon$ model* and the *shear stress transport $k-\omega$ model ($k-\omega-sst$)* were selected to govern the turbulence viscosity characteristic. These models have been proven to be suitable with the supersonic flow field [16, 18]. In this study, both models were used to compare the accuracy of predicting steam ejector's performance.

The benefit of *realizable $k-\epsilon$ model* is that it accurately predicted the spreading rate of both planar and round jets. In addition, it was also likely to provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients and separation [16]. The benefit of *$k-\omega-sst$ model* was that it could predict free shear flow spreading rate that were closely agreement with measurement for far wakes, mixing layers, and plane, round and radial jets, and was thus applicable to wall-bounded flows and free flows.

4.2.4 Working fluid properties

Actually, the properties of working fluid (water vapor) should be based on real gas assumption, but it required very long time for calculation and it was difficult to reach its convergence criterion. However, the steam ejector was mostly operated at a relatively low absolute pressure. In this situation, the properties of the working fluid could be assumed to be based on ideal gas assumption [7]. Base on ideal gas assumption, the density of working fluid is evaluated by using ideal gas relation which can avoid the difficulties of iteration. The properties of working fluid (based on ideal gas assumption) for the simulation are shown in table 4.1.

Table 4.1: The working fluid properties

Properties	Value
Viscosity, (kg/m.s)	1.34×10^{-5}
Thermal conductivity, (W/m.k)	0.0261
Specific heat, (J/kg.K)	2014.00
Molecular weight, (kg/kmol)	18.01534

4.2.5 Boundary conditions

There are two types of boundary condition that was suitable for turbulence compressible flows: *pressure-inlet* and *pressure-outlet* type [16]. For the inlet of steam ejector (primary fluid inlet and secondary fluid inlet), the *pressure-inlet* type was applied to this face. For the outlet of steam ejector (mixed fluid outlet or subsonic diffuser), the *pressure-outlet* type was applied. The values of operating conditions were assigned as the saturation properties (both pressure and temperature).

The ejector's walls of model were set as adiabatic walls. This means that the heat loss at the wall boundary is neglected. This is done to avoid the complexity of heat transfer function to the mathematical model. It was also shown from a literature [4] that the adiabatic wall provided less impact to the ejector's performance.

4.2.6 Near wall treatments

In the case of CFD investigation based on *reliable* $k-\varepsilon$ turbulence viscosity model, the near wall treatment is necessary defined. This is because the flow close to the ejector's wall to be more realistic. In FLUENT 6.3, it provides three optional near wall treatments, *standard wall function, non-equilibrium wall function and enhanced 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. The enhanced wall treatment provides accurate prediction when the flow form is low-Reynolds number flows such as boundary layer separation flows, buoyancy-driven flows.

In the past studies [3], it was shown that non-equilibrium wall function was not in agreement with the results of the simulated static pressure profiles along the center line of the ejector compared with the experimental values. Meanwhile, the standard wall functions provided more accurate results. The enhanced wall function could predict the closest results to the experimental values. However, using the enhanced wall function, it required much more time for calculation than the others type of wall functions. In this case, the standard wall function was preferable in order to investigate the steam ejector's performance. Even though, the errors provided by standard wall function were more than the enhanced wall function but these errors were acceptable. Moreover, it required much less time for calculation. Therefore, during the simulation, the *standard wall function* was selected to govern the near wall boundary layer.

For the case of CFD investigation base on $k-\omega$ -*sst* turbulence viscosity model, it is not necessary to define the near wall treatment. This is because the mathematical model of $k-\omega$ -*sst* is already emphasized the near wall treatment.

4.2.7 Convergence criteria and solution

This CFD simulation of the ejector model was considered as converged when the following two converging criteria were satisfied. Firstly, it had to be shown that the mass fluxes of every face in the model were stable. This means that it was based on the conservation of mass. In this case study, the difference of mass flow rate inlet and outlet the ejector's model was less than 10^{-7} kg/s. Secondly, every type of the calculation residual must be reduced lower than the specified value (in this case, less than 10^{-6}) in order to

ensure that the solution from simulation was accurate. During the simulation, the number of iteration for simulation was greater than 100,000 iterations. The mass flow rate of primary stream and secondary stream were considered as the entrainment ratio of steam ejector.

After the CFD technique of each simulation was considered as converged, these significant types of the solution data could be presented as:

- the entrainment ratio of steam ejector
- the filled contour of Mach number represent the flow inside the ejector

The entrainment ratio (R_m) 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 primary nozzle's inlet face. These mass fluxes can be directly determined in FLUENT.

4.10 Conclusion

In this chapter, the background of the CFD technique was introduced. The criteria of creating the calculation domain, grid element, and the information of the CFD ejector model setup (fluid properties, solver selection, turbulence model and boundary condition) including convergence criteria were provided.

The physical model was created as 2-D axisymmetric model and grid structure was created in the form of normal quadrilateral of 44,000 elements. The *density-based implicit* was used as a solver. Two turbulence viscosity models, *realizable $k-\epsilon$ model* and *$k-\omega$ -sst* were used. The detail of CFD model setup was summarized as shown in the table 4.2.

Table 4.2: The detail of the steam ejector's model

Criteria of steam ejector model	Specified criteria
Physical model	2-D axisymmetric
Boundary conditions	
- Upstream of the model	Pressure-inlet type
- Downstream of the model	Pressure-outlet type
Grid elements	44,000 structured quadrilateral
Solver setup	Density-based implicit
Turbulence viscosity model	Realizable k- ϵ and k- ω -sst
Working fluid	Water vapor base on ideal gas assumption
Near wall treatment	Standard wall function
Convergence criteria	Calculation residual is less than 10^{-6}