Numerical Modeling of Non-Equilibrium Condensing Steam Flows



# Numerical Modeling of Non-Equilibrium Condensing Steam Flows

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### Abstract

Two-phase condensing flows are very common in many technical applications, such as rotating machinery operating with steam and nuclear reactors. The occurrence of condensation can lead to a degradation of a component's performance. Thus, the physical understanding and accurate numerical modeling of the condensation process can be of great help in the design process.

The present work is focused on the numerical modeling of non-equilibrium condensing steam flows in 1-D nozzles. The fluid dynamic equations for an inviscid and adiabatic flow (Euler equations) are solved using a quasi 1-D finite volume code, which accounts for the nozzle area variation. The model for homogeneous nucleation and the droplet growth rate, presented by Dykas [26] in high-speed supersonic nozzle flow and also applicable to the wet stages of a steam turbine, is implemented in the present work. The model is based on the Eulerian-Eulerian method, i.e., the governing equations for both vapor and the liquid phase are based on an Eulerian frame of reference. The present work assumes an averaged pressure for both phases, with no slip condition between them. Hence, a single pressure and velocity characterizes the flow. The explicit first order accurate forward Euler scheme is used to advance the solution in time, until a steady state solution is reached. The convective fluxes are discretized using the Approximate Riemann Solver  $AUSM^+$  of Liou [4]. The classical nucleation theory proposed by Bakhtar and Young [5] provides the theoretical background for the modeling of condensing steam flow along with the growth of liquid phase.

The real gas behavior of the steam is taken into account using a cubic equation of state of iPRSV type (Peng-Robinson cubic equation of state with the Stryjek-Vera modification), as implemented in "FluidProp" [7] [8]. To model the non-equilibrium thermodynamics associated with the condensing flows a mixture model is used, i.e., the individual phases (vapor and liquid) are assumed to be a flowing mixture. This implies that properties such as enthalpy, entropy, internal energy and speed of sound are described in terms of a weighted average using the wetness fraction. The fluid dynamic system of equations is extended with two additional scalar equations with source terms to incorporate the condensation phenomenon in the flow field.

In order to assess the accuracy of the condensation model implemented, experimental data of various 1-D supersonic nozzle is compared to the numerical results. It is found that the

surface tension of the spherical liquid droplet has a significant effect on the accuracy of the results given by the nucleation model. It is concluded that the implemented numerical model is able to capture the condensation shock and compute the droplet size well within reasonable accuracy.

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### Nomenclature

### **Greek letters**

- $\alpha$  constant in AUSM<sup>+</sup>
- $\beta$  constant in AUSM<sup>+</sup>
- $\delta \qquad \qquad {\rm delta}$
- $\lambda_v$  thermal conductivity of vapor(W/m K)
- $\mu_v$  dynamic viscosity of vapor(Pa.s)
- $\rho$  density of mixture(Kg/m<sup>3</sup>)
- $\rho_v$  density of vapor(Kg/m<sup>3</sup>)
- $\rho_l$  density of liquid(Kg/m<sup>3</sup>)
- $\sigma$  surface tension(N/m)
- $\Psi$  variables vector AUSM+
- $\tau$  characteristic time(s)

### Latin letters

SOS E	speed of sound of $\text{IIIXture}(\text{II/S})$
	specific total internal energy of $mixture(J/Kg K)$
e $\mathbf{F}^n$	specific internal energy of $mixture(J/Kg/K)$
$\mathbf{F}$	euler nux vector
$\mathbf{F}^{(e)}$	convective wave
<i>F</i>	flux function
h M	enthalpy of mixture(J/Kg)
M m	Mach number
2010	variable of AUSM <sup>+</sup>
Γ	source term
P	averaged static pressure(Pa)
$P_s$	saturation pressure(Pa)
$\mathfrak{P}$	variable of AUSM <sup>+</sup>
R	specific gas $constant(J/Kg K)$
S	supersaturation ratio
Т	temperature (K)
$T_s$	saturation temperature(K)
t	time (s)
$\mathbf{Q}$	conserved variables vector
J	nucleation rate per unit volume $(m^{-3}s^{-1})$
K	Boltzmann's constant (= $1.3807 \times 10^{-23}$ J/K)
m	mass of a molecule of water (= $2.99046 \times 10^{-26} Kg$ )
Kn	Knudsen number
r	radius of droplet(m)
$r^*$	Kelvin-Helmholtz critical radius of droplet(m)
$q_c$	condensation coefficient
C	non-isothermal correction factor
y	wetness fraction
$g_{\tilde{z}}$	g-mer(number of molecules in a cluster)
ī	mean free path
$\Delta G$	change in gibb's free energy(J/Kg)
s	entropy(J/Kg K)
u	velocity(m/s)
$\gamma$	specific heat ratio
Nu	Nusselt number
$C_p$	specific heat at constant temperature(J/Kg K)
$\frac{dr}{dt}$	growth rate of droplets(m/s)
$\overset{al}{N}$	number of droplets per unit volume $(m^{-3})$
$\Delta T$	subcooling(K)
$C_{g}$	molecular rate of condensation on a g-mer
$E_q$	molecular rate of evaporation on a g-mer
$f_g$	concentration g-mers in supersaturated vapor

### Subscript

i-1	left control volume
i + 1/2	face
i + 1	right control volume
v	vapor phase
l	liquid phase

### Acronyms

ARS	Approximate Riemann solver
AUSM	Advection upstream splitting method
CFD	Computational fluid dynamics
CFL	Courant Friedrichs Lewy
EoS	Equation of State
MEoS	Multiparameter equation of state
iPRSV	improved Peng-Robinson-Stryjek-Vera
LPT	Low Pressure Turbine
1-D	One Dimensional

\_\_\_\_\_

## Chapter 1

## Introduction

This chapter gives a brief introduction on the motivation and objectives of the present work. Discussion is done on the relevance of this study, with respect to its applications. A brief outline of the phenomenology of the process of condensation and an outline of the work concludes the chapter.

### 1.1 Purpose and Motivation

Comprehensive understanding of condensing flow in various technological and environmental process is of utmost importance and also a major concern for many design engineers. Condensation is the process when water vapor changes from a gaseous to a liquid state. With reference to the environmental application for example weather prediction requires numerical solution of condensing flow and is discussed in detail by Thomas [42], Kristjansson [43] and Sundqvist [44]. Cloud formation, foggy mirrors and foggy windshield are other forms of condensation that find place in our daily life. In technical applications condensing flow have their presence in industries like nuclear [45] [46], turbomachinery [1] [27], pharmaceutical (production of sprays), and in chemical engineering during gas drying and flue gas cleaning. Accurate description of the flow involving condensation is challenging for designers and scientists due to the high complexity of the process and lack of advanced experimental techniques to measure every detail involved.

Spontaneous condensation that is initiated by homogeneous nucleation process is a common phenomenon in various applications. The homogeneous nucleation involves formation of metastable clusters (nuclei) of liquid due to fluctuations resulting from chance molecular collisions [37]. For example, condensation resulting from high humidity can cause inadequate ventilation in house. In steam turbines, condensing flow lead to corrosion and erosion of blades, wetness loss that results in loss of performance efficiency and change in flow pattern [1]. The success of all these applications relies on predicting and controlling the condensation process. Therefore it is important to understand the physical mechanism of the condensation process [37].

As discussed, homogeneous nucleation plays a role in various industrial applications. However, in the present study the motivation behind studying spontaneous condensation resulting from homogeneous nucleation is the fact that, formation of condensate in steam turbines leads to complex flow field leading to reduced performance efficiency. Figure 1.1 shows the wetness fraction contours obtained by Guha & Young [47] in a turbine blade, due to non-equilibrium condensation. Majority of the world's electricity demand is fulfilled from the steam propelled turbines. Hence, increase in the efficiency of the steam turbines will result in increase of the revenue generated, due to its long life term. In a Carnot cycle, an increase in efficiency can be attained by increasing the change in enthalpy across the steam turbine. However, this increased enthalpy change results in the expansion of the steam in the wet region (two phase region). The wet steam results in complex flow characteristics in the last stages of the Low Pressure Turbines (LPT). The wetness in steam is reduced, to a certain degree, through the reheating cycles, which increases the temperature of the steam entering the LPT. The use of reheating cycles requires huge investment costs. This fact has attracted interests of scientists and engineers in understanding the fundamental processes that leads to losses in steam turbines during the condensation process (wet steam), to help the steam turbine manufacturers with an improved design.

From this point of view, the present work is focused on understanding the homogeneous nucleation process that triggers condensation process. To understand this phenomenon it is chosen to study the expansion process of steam in supersonic nozzles from the dry superheated conditions to the wet steam conditions. The accurate modeling of condensing flows in nozzles depends on the quality of nucleation and droplet growth theories [37]. Therefore, objective of the present study is to gain physical insight on modeling of the nucleation and the growth theories. In order to accomplish this goal, the approach of this work has been to exploit the knowledge of classical nucleation theory laid down by Young & Bakhtar [5], along with droplet growth theories developed by Gyarmathy [14] [17] and Hertz Knudsen [16] [15].

Also the motivation behind this study is to extend the in-house CFD code, developed by Dr. Ir. Rene Pecnik at Stanford University under the Predictive Science Academic Alliance Program, funded by the Department of Energy, to the two phase flows. To fulfill this objective we implement and asses an in-house CFD code that is able to predict the spontaneous condensation accurately. The present work will primarily focus on the non-equilibrium condensation, whereby homogeneous nucleation is playing the major role. The following tasks, relating to modeling of condensing steam flow in rapidly expanding supersonic nozzle, have been dealt in this work:

- Theoretical understanding of non-equilibrium condensation process through comprehensive literature study.
- Accurate modeling of condensation process with the help of classical nucleation theory, i.e., homogeneous nucleation and droplet growth theory.
- Assessing the implemented code for its accuracy in predicting phenomena associated with condensation like, the droplet diameter, wetness fraction, nucleation rate and pressure distribution.
- Assessing the effect of surface tension of the spherical liquid droplets on the accuracy of the model.



**Figure 1.1:** Wetness contour in Low Pressure Turbines resulting from Non-Equilibrium Condensation [47].

- Selection of a robust droplet growth rate equation that is applicable for different Knudsen flow regimes.
- Implementation of a suitable Equation Of State (EoS) that is able to predict accurately thermodynamic states of vapor and liquid phase in metastable region.
- Selection of a suitable type of Approximate Riemann Solver (ARS) to calculate convective fluxes.

### 1.2 Thesis Overview

To achieve the objectives mentioned earlier, we will be focusing on providing a theoretical database for the modeling of condensing steam flow. Subsequently this model is implemented in an in-house CFD code and is assessed for its accuracy through comparison with experimental results.

Chapter 2 gives an extensive literature study on the phenomenon of spontaneous condensation. In this section the spotlight is on the theoretical as well as experimental work that has been carried out in the past in the field of nucleation and droplet growth theory. A comprehensive study of the classical nucleation theory and the droplet growth theory forms theme of this chapter.

Chapter 3 will detail the numerical methods and thermodynamic model used in the present research. The numerical techniques implemented to model complex thermodynamics of non-equilibrium condensation process is explained in detail. The numerical discretization scheme, which is important part of any CFD code is the center of focus of this section along with the thermodynamic EoS used.

Chapter 4 presents the results obtained by using the implemented model. Followed by discussion about the results obtained and how accurate they are with respect to the experimental studies.

Chapter 5 presents the conclusions and recommendations of the dissertation to further develop the present work.

## Chapter 2

## **Physical Modeling**

This chapter focuses on the thermodynamic and physical modeling of homogeneous nucleation and the droplet growth, which play a primary role in the condensation process. The goal of this chapter is to provide the reader with a comprehensive overview of the life history of droplets, i.e., the way droplets are born, grow in number and size. Moreover, special attention will be given to essential features and critical aspects of the physical modeling of the condensation process. It will be introduced here, the effect of surface tension of small spherical droplets on the performance of the nucleation models, especially when the cooling rate is high.

### 2.1 Overview of Condensation Theory

A comprehensive amount of literature is available for the modeling of non-equilibrium condensing flow. In the present work, focus is mainly on understanding the physics governing the phenomenon of spontaneous condensation and identifying the specific problems, to model it numerically. For this matter, a major part of the literature study was focused on understanding the nucleation theory and various growth models developed in the past.

The first observation of two shock-like disturbances in the supersonic airflow wind tunnels took scientists to surprise. Prandtl [9] was the first scientist to present the visuals of these shock like disturbances. It was Wieselberger who suggested the possibility of the presence of water vapor in the airflow that lead to shock like disturbances. Finally Hermann [10], after thorough and taxonomic investigations came to the conclusion that these shock like disturbances were indeed caused by the formation of water vapor in the air flow. Modeling of condensing flow was performed by Gyarmathy and Mesyer [12] and Hill [13], but it was Oswatitsch [11] in 1942 who suggested that the non-equilibrium condensation must be classified in two different processes, namely homogeneous nucleation and droplet growth. Oswatitsch [11] with Head [48], and Lukasiewicz and Royle [49] contributed to a detailed understanding of these processes through their experiments. They established empirical correlations between relative humidity, nozzle geometry and condensation onset [37].

Initially, the modeling of condensing flow was based on one-dimensional Laval nozzles, for which experimental data were more easily available. This was further followed by more sophisticated and advanced experiments by Barschdorff [18] on 1-D nozzle. Skillings et al. [19] were able to measure the droplet sizes in pure steam nozzles. Also, the experiments of Moore et al. [20] represents a valuable data set for the numerical codes validation. Hill [13] analyzed the data on condensation in supersonic nozzle and compared it with the predictions made by the nucleation and the droplet growth theory. Hill was the first to introduce an appropriate droplet growth theory for accurate theoretical predictions.

### 2.2 Condensation Modeling

In this section, thermodynamic aspects are introduced, which are imperative for the condensation process in supersonic nozzle flow. This is followed by detailed discussion about the classical nucleation theory and the droplet growth theory, which are characteristic part of a condensation process.

#### 2.2.1 Thermodynamic aspects

The simple definition of the condensation phenomena as, "the process of water vapor changing from a gaseous to a liquid state", is a prejudice of the complex physics involved during the phase transition [3]. The phase transition in condensation is associated with formation of the new surface between the vapor and the liquid phase. To form this new surface, an energy barrier has to be crossed. The transition to liquid state is preceded by nucleation. The phenomenon of nucleation is defined as the formation of small clusters of liquid phase within the vapor. The process of nucleation is thus crucial for the understanding of the dynamics of phase transition. Nucleation can occur in two different ways, homogeneous and heterogeneous. The homogeneous and heterogeneous nucleation can be distinguished from each other by the way two are initiated. The homogeneous nucleation produces its own stable clusters (nuclei) of liquid droplets, overcoming minimum energy barrier (Gibb's free energy), in the supersaturated vapor. Whereas heterogeneous nucleation requires foreign particles, that act as condensation nuclei, to activate the condensation process [3]. It is important to note that the minimum energy barrier associated with the heterogeneous nucleation is much lower than that of the homogeneous nucleation. This implies that for equal nucleation rate a much higher level of supersaturation<sup>1</sup> in the vapor phase is required for homogeneous nucleation than for heterogeneous nucleation. As a consequence, heterogeneous nucleation is usually encountered in nature around us like in the formation of atmospheric clouds. Whereas homogeneous nucleation is seen in engineering applications, for example in the high-speed nozzle flow or in the steam turbines. The condensation of steam is initiated in principle as soon as the thermodynamic state of the fluid crosses the saturation line in the Mollier diagram. However, this is not the case in practical applications, for example, homogeneous condensation in a transonic or supersonic nozzle flows. When the fluid expands through a supersonic nozzle, due to the rapid cooling, the vapor phase departs from the equilibrium phase distributions. The vapor phase will not condense immediately and attains a high degree of supersaturation, which is an indication that the vapor phase has attained a metastable equilibrium state [37]. Thus, the

<sup>&</sup>lt;sup>1</sup>For definition of Supersaturation please refer to 2.2.2

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process of condensation occurs under non-equilibrium conditions. The assumption of equilibrium state will lead to serious inaccuracies in predicting the flow behavior. The reversion back into the equilibrium state happens via the formation and growth of liquid droplets. The time period of the metastable state will depend on the degree of supersaturation the fluid has attained. During this time period of the metastable state, steam will expand in the nozzle as dry supersaturated vapor. As stated earlier, for the homogeneous nucleation to occur, the fluid needs to attain a high degree of supersaturation (e.g. typically for steam flows 30-40 °C supercooling <sup>2</sup> is required). No disturbance in the flow is observed during the homogeneous nucleation, when exceed some critical size, results in the growth of the liquid droplets. As shown in figure 2.1, between the points 4 and 4' the vapor is in metastable equilibrium state and is thus referred to as metastable region. The loci of the limiting points 2' and 4', where  $(\partial p/\partial v)_T = 0$ , are called liquid and vapor spinodals, respectively. Since the states along the path 2'-3-4' are not in equilibrium condition, the equations of state are not valid to describe them [64].

During the droplet growth process, a significant amount of latent heat is released in the flow. This heat release results in compressive effects that lead to the appearance of a shock thus interrupting the nucleation process, and ultimately leading to the formation of a stable liquid phase. The growth of these droplets occur in a deterministic way as a result of steady influx of vapor molecules that is captured from the supersaturated vapor phase. This will then cause a decrease of the vapor pressure, and a corresponding decrease of the supersaturation. Release of the latent heat causes both the droplet and the vapor temperatures to rise [3], and hence has a strong impact on the flow pattern. If the amount of latent heat released at a certain location in the nozzle exceeds the critical amount, the flow becomes thermally

<sup>&</sup>lt;sup>2</sup>For definition of supercooling please refer to 2.4.



**Figure 2.1:** p-v(Pressure-Volume) diagram for a pure substance illustrating metastable equilibrium [64].

choked and a steady shock appears in the nucleation zone. If this released heat is below the critical amount then a local increase in the pressure, temperature, Mach number and density appears. The former type of flow is referred to as supercritical flow, whereas the latter is termed as sub-critical flow.

Regarding the droplets, it is important to understand that the droplets size has a wide variation in scale and they typically start at the nanometer size  $(10^{-9}\text{m})$ , and eventually grow to micrometers  $(10^{-6}\text{m})$ . The numerical models used for describing the process of condensation for this wide range of droplet spectrum, the motion of the droplets, as well as the droplet-droplet interactions (e.g. coalescence), need to be assessed carefully for their accuracy [3].

The relaxation gas dynamics forms the framework for the understanding of non-equilibrium condensation. Thus, the relaxation times of the internal rate processes is a key parameter in the understanding of non-equilibrium condensing flows and this will be discussed in sections to follow.

#### 2.2.2 Supersaturation

Supersaturation is the inability of a fluid to condense when the saturated condition is reached in an expansion. The theory of supersaturation explains the phenomenon involved in the flow of the saturated or wet steam in a supersonic nozzle. It is observed that steam will not begin to condense when the saturated condition is reached, while undergoing very fast expansion through a supersonic nozzle from the dry conditions. The steam continues to expand in the nozzle as dry vapor, thus becoming supersaturated. Such a theory explains the excess flow encountered in the expansion of a saturated steam through nozzles [1]. Supersaturation is formulated in terms of the supersaturation ratio S and is defined as the ratio of vapor pressure P to the saturation pressure corresponding to the local vapor temperature  $P_s$  ( $T_v$ ). This parameter is a measure of the degree of supersaturation, the vapor has achieved and is defined by the equation (2.1)

$$S = \left[\frac{P}{P_s(T_v)}\right].\tag{2.1}$$

Supersaturation is also a measure of the departure of the fluid from thermodynamic equilibrium. Henderson [54] observed that the amount of steam discharged in the Laval nozzles, from the dry region into the wet region in the Mollier chart for non-equilibrium conditions was approximately 5% greater than the value that would be expected from equilibrium calculations. The Wilson line is defined by the limiting supersaturation, i.e., at the termination of the supersaturated state of the vapor. It is important to know the location of the Wilson line, which is an indication of the condition at which condensation actually begins. The Wilson line, named after the scientist G. T. R. Wilson, on the Mollier chart marks the limit of supersaturation. Wilson was able to measure the pressure at which condensation actually begins by expanding the air saturated with moisture in a glass chamber. From this he deduced the supersaturation ratio. It was found by Johni Yellott [28], that in a simple Laval nozzle condensation did not occur until the steam had reached the condition approximately represented by the 3.5 % moisture line on the Mollier chart. The theory introduced by Yellott [28] is useful to understand supersaturation. The vapor pressure of a liquid at a given temperature is greater over a curved surface than over a plane surface. In figure 2.2 (a), it can be seen



Figure 2.2: Vapor pressure above plane and curved surface [28].

that a molecule x resting on a flat liquid surface is attracted by all the molecules of the liquid within the radius of p, the distance over which the molecular attraction acts. Whereas, in figure 2.2 (b), a molecule y resting on a curved surface is attracted by fewer molecules than x. Thus at the same given temperature, molecule y is tied less securely to the surface than molecule x. This implies that a greater pressure in the atmosphere surrounding molecule y will be required to force y to remain on the surface, than that at x. In other words, the vapor pressure in case (b) is greater than that in (a). Thus a water droplet, if sufficiently small, will evaporate if placed in an atmosphere of saturated steam. However, if the vapor is supersaturated or at a pressure greater than that corresponding to its temperature, equilibrium can exist between the vapor and the droplet when the pressure of the vapor is equal to the vapor pressure of the droplet [28]. The pressure of the supercooled vapor is always higher than the saturation pressure corresponding to its own temperature. Thus the supersaturation ratio S of a supercooled vapor is will always be greater than 1.

The mechanism of the droplets formation will now be discussed in detail. In the present study, it is assumed that the droplets are spherical in shape. As said earlier, in order to promote the formation of droplets and their further growth, the required surface has to be formed by molecular clusters (small embryo of a liquid droplet) and therefore supply of a surface free energy and decrease of bulk free energy of transition from the vapor to liquid is necessary. The change in Gibb's free energy  $\Delta G$ , during the formation of a single spherical droplet from the supersaturated vapor held at constant pressure P and temperature  $T_v$ , is given by equation (2.2)

$$\Delta G = 4\pi r^2 \sigma - \frac{4}{3}\pi r^3 \rho_l R T_v \ln S.$$
(2.2)

The free energy change could be described in following five steps:

Step-1: Formation of the first "n" molecules from the superheated steam. There is no change in free energy during this process

$$\Delta G_1 = 0. \tag{2.3}$$

Step-2: Isothermal expansion of steam from pressure P to saturation pressure  $P_s(T_v)$ 

$$\Delta G_2 = \frac{4}{3}\pi r^3 \rho_l \int_P^{P_s} \frac{1}{\rho_v} dp = -\frac{4}{3}\pi r^3 \rho_l R T_v \left[\frac{P}{P_s(T_v)}\right],$$
(2.4)

where,  $\frac{P}{P_s(T_{v})} = S$ .

Step-3: Condensation of the "n" molecules of vapor at saturation pressure  $P_s(T_v)$  and constant temperature  $T_v$  into bulk liquid, and creation of a flat surface. On account of equilibrium

between the two phases and since their chemical potential is equal, the free energy remains unchanged

$$\Delta G_3 = 0. \tag{2.5}$$

Step-4: Formation of droplets of radius "r" and surface of area,  $4\pi r^2$ , the free energy change of droplet increases to

$$\Delta G_4 = 4\pi r^2 \sigma, \tag{2.6}$$

where,  $\sigma$  is the surface tension of the spherical liquid droplets.

Step-5: The droplets thus formed are isothermally compressed from the saturation pressure  $P_s(T_v)$  to the vapor pressure P. The liquid phase volume and the radius of the droplets will not change due to the assumption of incompressibile fluid. Thus, the free energy change is

$$\Delta G_5 = \frac{4}{3}\pi r^3 (P - P_s). \tag{2.7}$$

This last contribution,  $\Delta G_5$  is neglected as it is very small in magnitude compared to other contributions in change of Gibb's [5].

Summing all the partial changes of the free energy leads to equation (2.2). The first term in the equation (2.2) represents the increase in free energy due to the formation of liquid bulk surface, while the second term represents the increase in free energy due to formation of the interphase between vapor and liquid. From equation (2.2) it can be seen that for a supersaturated vapor, S >1, the first term will be always positive while the second term is negative. However, for the small droplets of radius r first term dominates. From figure 2.3, plotted for various supersaturation ratios, it can be seen that for a given supersaturation ratio,  $\Delta G$  increases with radius r of the droplet and reaches a maximum value  $\Delta G^*$ . The radius of droplet corresponding to this maximum value  $\Delta G^*$  is termed as the Kelvin-Helmholtz or critical radius,  $r^*$ . A droplet with  $r \geq r^*$  can reduce the free energy of the system by capturing



**Figure 2.3:**  $\Delta G$  versus r for various supersaturation ratio [1].

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molecules, and has a tendency to grow. While a droplet with  $r < r^*$  evaporates. Equation (2.2) reveals that the free energy change is dependent on droplet radius "r". An expression for the critical radius  $r^*$  is obtained by differentiating equation (2.2) with respect to r and equating it to zero, which gives the equation (2.8)

$$r^* = \frac{2\sigma}{\rho_l R T_v \ln(S)}.$$
(2.8)

This critical cluster of molecules with radius  $r^*$  is always in metastable equilibrium with the vapor surrounding it. It is clear that by increasing the supersaturation ratio S, the activation barrier  $\Delta G^*$  and the size of critical clusters  $r^*$  decreases, which is also evident from figure 2.3. In other words, increasing the supersaturation ratio S will increase the probability that molecular clusters can overcome the free energy barrier  $\Delta G^*$  and nucleation can be triggered. At this moment, homogeneous nucleation will start and phase transition can finally take place.

#### 2.2.3 Classical Nucleation Theory

The expression for the nucleation rate J that forms the backbone for numerical modeling of the non-equilibrium condensing flow will be discussed in this section. Historically the theories of homogeneous nucleation have developed on two lines, one being the thermodynamic-kinetic approach while the other is based on statistical mechanics and is being formed to eradicate the uncertainties that surround the classical theory. The theoretical developments to understand nucleation and droplet growth have been supported by experimental activities, primarily in Laval nozzles. However, in the past the only data that scientist were able to measure was the centerline pressure distribution in Laval nozzles. This information was then used to infer the limiting supersaturation in high-speed nucleating flows. Information regarding the pressure distributions in Laval nozzle can be used to compare with the results obtained by numerical solution of the conservation equations describing droplet nucleation and growth combined with the gas dynamic conservation equations [5]. However, only the information about the pressure distribution is not sufficient to understand the uncertainties associated with nucleation theory. Better experimental techniques and optical techniques were developed for measuring the droplet size (Deych et al. [29], Stein [30], Gyarmathy and Lesch [31] and Walters [32]). Wyslouzil et al. [33] further developed the techniques to measure the size and structure of the extremely small droplets (size of nano scale order) by the use of small-angle neutron scattering. This development made it possible to fetch more accurate information about small clusters of molecules formed by the process of homogeneous nucleation. This can be used to validate nucleation theories and hence made it possible to validate numerical solutions of condensing flows more accurately. As addressed by J. Young and F. Bakhtar [5] that classical nucleation theory explains qualitatively the process of nucleation in a steam nozzle quite well. However it lacks quantitative accuracy and hence more work in this direction is required.

From the knowledge of elementary thermodynamics and kinetic theories an expression for the nucleation rate can be formulated. This expression is a function of the thermodynamic state of the vapor. As stated earlier, in a supersaturated vapor the process of cluster formation occurs if the clusters exceed the critical size and encounter a favorable  $\Delta G$  gradient. It is to be noted that the steady state assumption is no longer applicable because the rate at which the clusters grow and decay is not balanced. A droplet of radius r comprising of g molecules

is called a g-mer. The net rate per unit volume  $I_g$  at which g-mers grow to (g+1)-mers is termed as the nucleation current and is expressed by equation (2.9)

$$I_g = C_g f_g - E_{g+1} f_{g+1}, (2.9)$$

where  $C_g$  is the rate at which a cluster acquires a molecule (the condensation rate),  $E_{g+1}$  is the rate at which cluster loses a molecule (the evaporation rate) and  $f_g$  denotes the concentration of g-mers.

The time rate of change of the concentration of g-mers is then given by expression (2.10)

$$\frac{\partial f_g}{\partial t} = -\left[ (C_g f_g - E_{g+1} f_{g+1}) - ((C_{g-1} f_{g-1} - E_g f_g)) \right] = -(I_g - I_{g-1}) \cong -\frac{\partial I_g}{\partial g}, \qquad (2.10)$$

 $C_g$  can be obtained from the kinetic theory expression for the rate at which vapor molecules impact the droplet surface. Assuming that clusters can be modeled as spherical droplets down to the smallest sizes [5].

$$C_g = q_c A g^{\frac{2}{3}} \frac{\rho_v \bar{\nu}_v}{4m},$$
(2.11)

where  $\bar{\nu_v}$  is the mean speed of vapor molecules and  $q_c$  is the condensation coefficient, the fraction of molecules incident on the surface that are absorbed into the droplet.

The solution of equation (2.10) is obtained such that we eliminate the  $E_{g+1}$  term. To do this we will first solve equation (2.9) and will eliminate  $E_{g+1}$  term from it, thereby we get

$$\frac{I_g}{C_g n_g} = \frac{f_g}{n_g} - \frac{f_{g+1}}{n_{g+1}} \cong -\frac{\partial}{\partial g} \left(\frac{f_g}{n_g}\right).$$
(2.12)

Where  $n_g$ , is the number per unit volume of g-mers and is expressed as

$$n_g \cong n_1 exp\left(\frac{-\Delta G}{KT_v}\right),\tag{2.13}$$

and  $n_1$ , is the number per unit volume of monomers. It should be acknowledged here that  $n_g$  does not represent real distribution of g-mers and is just a mathematical trick to eliminate  $E_{g+1}$ .

Eliminating  $I_g$  from equations (2.10) and (2.12), the time rate of change of the cluster concentration is given by following expression in differential form

$$\frac{\partial f_g}{\partial t} = -\frac{\partial I_g}{\partial g} = \frac{\partial}{\partial g} \left[ C_g n_g \frac{\partial}{\partial g} \left( \frac{f_g}{n_g} \right) \right]. \tag{2.14}$$

Equation (2.14) is the transport equation describing isothermal nucleation, i.e., there is no temperature difference between the droplets and vapor. The solution of equation (2.14) for isothermal nucleation is carried out in two distinct ways: steady state or in transient state. Kashchiev [50] investigated the solution of equation (2.14) in transient state in terms of a characteristic time  $\tau$ . If a given supersaturation is imposed on a vapor initially in a saturated condition, then  $I_g$  reaches 99 % of its steady state value within a characteristic time of  $10^{-7}$  to  $10^{-6}$  s [50]. Calculations show this time scale to be very short in comparison with the overall time for active nucleation in nozzles [5]. Thus, transient state is usually neglected in

condensing flow calculations and it is assumed that steady state nucleation rate is attained instantaneously. For the steady state solution, equation (2.12) can be integrated as

$$J_{CL} \int_{g=1}^{\infty} \frac{dg}{C_g n_g} = \int_{g=1}^{\infty} -d\left(\frac{f_g}{n_g}\right), \qquad (2.15)$$

where  $J_{CL}$  is the classical steady-state value of I. Evaluating the integral on the right-hand side

$$J_{CL} = \left\{ \int_{g=1}^{\infty} \frac{dg}{C_g n_g} \right\}^{-1}.$$
 (2.16)

The integral in equation (2.16) is solved analytically. Complete solution of this integral is provided in Appendix-A giving final expression for nucleation rate as

$$J_{CL} = q_c S \frac{\rho_v^2}{\rho_l} \left(\frac{2\sigma}{\pi m^3}\right)^{\frac{1}{2}} exp\left(-\frac{4\pi r^{*2}\sigma}{3kT_v}\right).$$
(2.17)

It is observed that the nucleation rate J is negligibly small, even at low or moderate supersaturation ratios S, but it rises perilously with an increase in  $\Delta T = T_{sat} - T_v$ , as shown in figure 2.4. The above expression for nucleation rate is taken from the classical theory. There has been some key developments in this theory that is incorporated in present work. These developments are stated below:

- Courtney's correction: Courtney [34] had proposed the first correction to the classical nucleation theory. He observed that the effect of the partial pressure of the clusters for g-mers>1 had been omitted from the classical theory. Courtney's correction reduces the expression for the classical nucleation rate (2.17)  $J_{CL}$  by a factor S (supersaturation ratio). The classical form for  $\Delta G$  is inconsistent with the law of mass action whereas the one revised by Courtney is.
- Condensation coefficient: The condensation coefficient  $q_c$  appears in the nucleation rate equation. Most authors like Mozurkewitch [52] calculated the value of this coefficient in a range close to unity. Mills [51] performed experimental investigation to determine the inter-facial heat transfer resistance, in order to calculate condensation coefficient of water. Mills through his experiment found that the inter-facial heat transfer resistance was not significant and the values of the condensation coefficient varies in the range of 0.45 to unity. Moreover Millikan [53] proved with a classic oil drop experiment that about 90 % of incident molecules suffered diffusion, indicating that almost all of the incident molecules were absorbed. It should be noted here that the value of the condensation coefficient as unity is obtained by experiments on large surfaces. On the other hand for small clusters the condensation coefficient is less than unity. However, the non-isothermal correction of nucleation theory makes the nucleation rate almost insensitive to condensation coefficient value in a range of 0.1 to 1.0 [5].
- Non-Isothermal Effects: The classical theory is based on isothermal assumption, i.e., the vapor and droplet temperature are equal. During condensation, however, latent



**Figure 2.4:** Variation of the classical nucleation rate per unit mass of vapor with supercooling at various pressures [5].

heat of vapor molecules in the nuclei is released. This heat has to be conducted to the surrounding vapor and is realized by gas kinetic collisions and not by macroscopic heat conduction. The reason is that the size of the critical nuclei is smaller than the mean free path length and the process occurs in the gas dynamic region. Due to this fact there is a temperature difference between the nucleus (liquid embryo) and the surrounding vapor, which is dependent on the amount of molecules condense or evaporate, and thus changing the thermal balance. The thermal non-equilibrium between the phases also affects the nucleation rate J [1]. Thus, Kantrowitz [35] formulated a simple correction to the isothermal classical theory of nucleation.

Applying the presented corrections to the classical form of the nucleation rate, a modified nucleation rate is formed. In the present model, in order to account for the relevant phenomena associated with process of homogeneous condensation, all three corrections mentioned above are applied to give a modified expression for nucleation rate as

$$J_{CL} = C \frac{\rho_v^2}{\rho_l} \sqrt{\frac{2\sigma}{\pi m^3}} exp\left(-\frac{4\pi r^{*2}\sigma}{3kT_v}\right),\tag{2.18}$$

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where C is a non-isothermal correction factor that is given by the following relation

$$C = \left\{ 1 + 2\frac{\gamma - 1}{\gamma + 1} \frac{h_v - h_l}{RT_v} \left( \frac{h_v - h_l}{RT_v} - \frac{1}{2} \right) \right\}^{-1}.$$
 (2.19)

We have derived the present equation (2.18) of nucleation rate in steady state conditions. It was described earlier that the characteristic time required for nucleation rate to reach the steady state is around  $\tau = 10^{-7}$  to  $10^{-6}$  s. In a typical nozzle flow, the cooling rate ranges from 0.2-0.8 K/ $\mu$  s with a temperature variation of less than 1 K in one microsecond. Thus, the temperature change during the nucleation process is insignificant. Moreover the flow field, in a nozzle, varies in time with a characteristic time period of typically  $\tau * = 10^{-3}$ s [37]. It can be observed that  $\tau *$  is three to four orders of magnitude higher than  $\tau$ . Therefore, the steady state nucleation rate derived by equation (2.18) is a good approximation and can be applied to both steady and unsteady flows in nozzles.

#### 2.2.4 Droplet Growth Theory

The small clusters of critical size of liquid may grow in the supercooled vapor as the vapor molecules condense further on the their surface. Flux of mass (vapor molecules) towards the droplet and net flux of energy (release of latent heat) to the vapor are characteristic behavior of the droplet growth process [37]. This latent heat transfer causes the vapor temperature to rise instantaneously. Consequently, the vapor pressure P rises during the initial growth process, also known as condensation shock. Thus, the growth rate of a droplet is a function of the heat transfer rate between the droplet and the vapor, and strongly depends on rate at which heat is conducted away from the droplets [1]. These mechanisms of heat transfer and mass flux to a great extent depends on the Knudsen number (Kn). The Knudsen number is defined as the ratio of mean free path of the vapor molecules to the droplet size, i.e., the droplet diameter and is expressed as

$$Kn = \frac{\tilde{l}}{2r},\tag{2.20}$$

where  $\tilde{l}$  is the mean free path of the vapor molecules given by expression

$$\tilde{l} = \frac{3\mu_v}{P} \sqrt{\frac{\pi R T_v}{8}},\tag{2.21}$$

where  $\mu_v$  is the dynamic viscosity of the vapor.

The Knudsen number plays a primary role in the heat transfer coefficient due to the existence of wide range of droplet radius formed during the process of condensation. For very small Knudsen number (Kn $\ll$ 1), the continuum hypothesis is applicable and the transfer process is governed by diffusion. Whereas, for large Knudsen number (Kn $\gg$ 1) kinetic gas theory is applicable (rarefied gas effects) and the process is governed by the kinetic process of impingement of the vapor molecules to the droplets [37]. Despite the large amount of literature on growth models with different levels of complexity to account for different regimes of Knudsen number, a universally applicable growth model has not been formulated. Different growth models proposed by various authors can be broadly classified into rarefied gas effects for transitional or diffusion controlled growths. In this respect, the Langmuir model is an interesting theory that takes into account both continuum and rarefied gas effects. As shown in figure

2.5, the region around the droplet is divided into two zones, i.e., the outer region and the inner region. In the outer region the continuum mechanics equations are applied, whereas in the inner region, termed as Knudsen layer, the transfer processes are governed by kinetic gas theory. For the flow inside nozzles, the Knudsen number varies in a wide range, from the continuum to the free-molecule regime. Hence Langmuir model finds the best fit in these applications. Figure 2.5 shows, Knudsen layer at a radius  $r + \beta l_g$ , which separates the continuum regime from the free molecular regime, where  $\beta$  is a constant of the order unity [1]. To formulate the rate at which the droplets grow, it is important to account for the coupling between mass and energy. Thus an energy balance around a spherical droplet or radius r is done and the following expression is obtained

$$m\frac{dh_p}{dt} = -(h_v - h_l)\,\dot{M} - \dot{Q}.$$
(2.22)

In equation (2.22), the term on left hand side is called sensible heating usually is small, owing to very small size of the droplets of liquid, and therefore can be neglected. The first term on the right hand side of equation (2.22) is the latent heat energy to be removed from the droplet. The second term is the convective heat transfer rate  $\dot{Q}$ .  $\dot{M}$  is the mass transfer rate given by

$$\frac{dm_p}{dt} = -\dot{M},\tag{2.23}$$

here  $m_p$  is the mass of a single spherical droplet expressed as

$$m_p = \frac{4}{3}\pi r^3 \rho_l.$$
 (2.24)

Substituting (2.23) and (2.24) in (2.22) we get

$$(h_v - h_l) \frac{dm_p}{dt} = 4\pi r^2 K_v \left( T_l - Tv \right), \qquad (2.25)$$



Figure 2.5: Langmuir model and Temperature distribution around a droplet [1].

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where  $\frac{dm_p}{dt}$  is the mass condensation rate over the surface of the droplet,  $(h_v - h_l)$  is the local latent heat per unit mass and  $(h_v - h_l)\frac{dm_p}{dt}$  is the rate of latent heat to be removed from the droplet. A part of the latent heat is convected to the vapor, while the remaining part is used to raise the droplet temperature. In the above expression,  $T_l$  represents the temperature of the liquid and is assumed to be equal to the saturation temperature  $T_s$  at the corresponding vapor pressure. Simplifying equation (2.25) by substituting the value for  $m_p$ , the droplet growth can be expressed as

$$\frac{dr}{dt} = \frac{K_v \left(T_s - Tv\right)}{\left(h_v - h_l\right) \rho_l}.$$
(2.26)

For the small droplets that are generated due to homogeneous nucleation, the heat transfer coefficient  $K_v$  must be modified to account for Knudsen (Kn) number effects. A heat transfer coefficient which includes this dependence, and that is appropriate for steam, was developed by Gyarmathy [12], and is expressed as

$$K_v = \frac{Nu\lambda_v}{2r} = \frac{\lambda_v}{r\left(1 + cKn\right)}.$$
(2.27)

The value of the constant c in the equation (2.27) was proposed by White and Young [21] to improve the agreement with experimental results at low pressures. Using Gyarmathy's approximation, equations (2.26) and (2.27) can be combined along with the definition of the Nusselt number to give the following expression for growth rate

$$\frac{dr}{dt} = \frac{1}{\rho_l} \frac{\lambda_v}{(1+3.18Kn)} \frac{(T_s - T_v)}{(h_v - h_l)} \frac{r - r*}{r^2}.$$
(2.28)

Detailed derivation of the above growth rate is given by Keramat Fakhari [1]. Equation (2.28) is termed Gyarmathy's droplet growth equation, which takes into account the diffusion of vapor molecules through the surrounding vapor. Another expression for droplet growth rate for the free molecular energy transfer rate between the droplet surface and the interface is given by Hill [13]

$$(h_v - h_l) \rho_l \frac{dr}{dt} = \dot{Q} = \frac{P}{\sqrt{2\pi r T_v}} \frac{\gamma + 1}{2\gamma} C_p (T_s - T_v).$$
(2.29)

Rearranging the terms in equation (2.29) we get to

$$\frac{dr}{dt} = \frac{P}{\left(h_v - h_l\right)\rho_l \sqrt{2\pi r T_v}} \frac{\gamma + 1}{2\gamma} C_p \left(T_s - T_v\right).$$
(2.30)

### 2.3 Surface Tension

Young [36] indicated the importance of testing the accuracy of nucleation and the droplet growth theory individually. To accomplish this goal, it is important to have the data for the pressure measurement and droplet size. This implies that the validation of any condensation model in calculating the non-equilibrium condensing flow is strongly dependent on the accuracy of the nucleation theory and the droplet growth theory. However the accuracy of the practical computation of the nucleation rate depends on the properties of the droplets with

small radius. The most important property, which has very strong effect on the nucleation rate is the surface tension [6][37]. It can be seen from the equation (2.18) that surface tension of the droplet appears in the exponential term and small inaccuracy in this value can result in a dramatic change of nucleation rate. The uncertainty associated with the calculation of surface tension of sub-cooled spherical water droplet seriously hampers the validation process of any condensation model.

It has been claimed by many scientist that the surface tension of a highly curved surface liquid may differ significantly from the surface tension of a bulk liquid with flat surface [38][39]. Tolman [39] used the results of Gibbs thermodynamic theory of capillarity to assess the effect of droplet size on surface tension. Tolman came to the conclusion that surface tension can be expected to decrease with decrease in droplet size. But this decrease in the surface tension is observed only in very small droplets (diameter of nanometer size). In other words, the Tolamn's theory states that there is no sensible effect of curvature of the droplets on surface tension in the macroscopic domain. The dependency of the surface tension on the droplet size and its extrapolation to the sub-cooled region has been a topic of debate. Since the critical droplet of nucleation theory represents a cluster of molecules of radius of the order of  $10\dot{A}$ , and is definitely outside the domain of applicability of macroscopic thermodynamic concepts [40]. Hence there is a need for the development of the nucleation theory whose dynamics can be extrapolated from macroscopic concepts into the microscopic domain without subjection to any ambiguities.

In the present work we have computed the surface tension  $\sigma$  as a function of temperature only. In order to calculate the surface tension, the vapor temperature  $T_v$  will be used instead of the liquid saturation temperature  $T_s(\mathbf{P})$  owing to the fact that the freshly formed liquid droplets are in equilibrium with the vapor around it. In the nucleation theory proposed in the earlier section it can be observed that the expression for nucleation rate J (2.18) contains other terms apart from surface tension, that are defined for corresponding thermodynamic equilibrium state. The equation formulated by Vargaftik et al. [41] is used to account for the temperature dependence of  $\sigma$ , and is expressed as

$$\sigma = B \left[ \frac{T_c - T_v}{T_c} \right]^{\mu} \left[ 1 + b \left( \frac{T_c - T_v}{T_c} \right) \right], \qquad (2.31)$$

where  $B = 235.8 \times 10^{-3}$  N/m, b= -0.625 and  $\mu = 1.256$  are empirical constants.

Equation (2.31) is an interpolating equation that is able to calculate the surface tension of water droplets within a temperature range of 0.01 to 374°C well within estimated uncertainties. This interpolating equation has been recommended by the International Association for the Properties of Steam (IAPS) and predicts the surface tension of water droplets quite accurately.

It was observed by Lai et al. [6] that only a small change in the surface tension resulted in a substantial change in the pressure distribution, nucleation rate, mean droplet radius and droplet size distribution. As a matter of fact, higher surface tension ratio (ratio of surface tension for spherical droplet to that for the flat surface) tends to give a smaller nucleation rate and a broader nucleation zone, which delays the onset of condensation process along with increase in the mean droplet radius. The results are relatively sensitive to the change in surface tension ratio.


**Figure 2.6:** Axial Pressure distribution in a convergent divergent nozzle with spontaneous condensation [27].

### 2.4 Condensation in Nozzles: A Summary

To summarize the present chapter an example on the process of condensation in a typical Laval nozzle, i.e., a convergent-divergent nozzle, is presented. Figure 2.5 shows expansion in a typical convergent-divergent nozzle starting from the superheated dry conditions into the wet conditions. From figure 2.5, at the point (1) steam enters the nozzle in the form of the dry superheated vapor. The steam is expanded to sonic conditions due to diverging geometry of the nozzle. From point (1) till the point (2) steam is in the dry superheated conditions and has not crossed the saturation line. It is only at the point (3), that the saturation line is crossed. The crossing of saturation line happens before or after the throat depending on the geometry of nozzle and expansion rate. The liquid droplet embryos (molecular clusters) begin to form and collapse in the vapor in this region. However, the rate of nucleation associated with these early embryos is very low, and hence the steam continues to expand as a dry vapor in a metastable sate. The nucleation rate increases instantaneously and reaches its maximum at the point (4). This peak in nucleation happens as the limiting supersaturation is reached,

indicated by the Wilson line in the figure. It is at this point that the onset of nucleation happens and thus this area is termed as nucleating zone and is terminated by the Wilson point, which is the point of maximum supercooling or supersaturation. Here supercooling is often used by engineers because of its more obvious physical significance. Supercooling is defined as the difference between the saturation temperature  $T_s(\mathbf{P})$  at the vapor pressure P and the vapor temperature  $T_v$ . It is often represented by symbol  $\Delta T$ .

$$\Delta T = T_S(P) - T_v. \tag{2.32}$$

After the point (4), nucleation ceases effectively and the number of droplets in the flow remains constant. It is only between the points (4) and (5) that these nuclei grows rapidly, helping the system to reach the thermodynamic equilibrium. Further expansion of the flow between the points (5) and (6) takes place close to the equilibrium conditions. While reaching to the stable thermodynamic equilibrium via a change of the phase, a release of latent heat to the vapor phase from the liquid phase happens. This release of heat causes a kink in the pressure between the points (4) and (5) indicating the process of condensation has occurred in the expanding flow. The process of this expansion can also be represented in an enthalpy-entropy (h-s) diagram as shown in figure 2.7.



**Figure 2.7:** State path for expanding steam with spontaneous condensation in Enthalpy-Entropy (h-s) diagram [27].

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# Chapter 3

# **Numerical Modeling**

This chapter presents the numerical schemes used to model the condensation phenomenon and implemented in an in-house quasi 1-D Euler solver. A detailed description of the equations governing the two-phase flow is presented. This is followed by the discussion of appropriate numerical methods for discretization of the governing equations for gas dynamics along with the Approximate Riemann Solver (ARS) required for discretizing the convective fluxes. It is also the objective of this chapter to incorporate the description of the equation of state used to model the real gas behavior of the steam.

### 3.1 Overview of the Numerical Studies

From fluid mechanics point of view, there are two universal descriptions of motion namely, the Lagrangian approach and the Eulerian approach. Many of the authors in the past have used a coupled Eulerian-Lagrangian approach to model the condensing flows accurately. In Eulerian-Lagrangian models the numerical modeling of liquid phase i.e. clusters of droplets, is done using Lagrangian approach and the trajectories of the individual particles is tracked. On the other hand equations for mass, momentum and energy were solved based on the Eulerian approach. The time-accurate calculations were used to investigate the self-induced oscillations in homogeneous condensing flows. In the Eulerian assumption the clusters of droplets is considered to be dense and therefore is regarded as continuum. In the Eulerian-Eulerian models commonly referred as two-fluid models, both phases are considered as a continuum. The selection of an appropriate model is governed by the nature of flow and the required level of accuracy. In the Eulerian model the fluid path from one cell to the next is not accounted for and hence the behavior of the fluid from the cell it has emerged is not necessary to be known. This property of the Eulerian model allows to develop equations in a time marching form and extension to three dimension is more straightforward. However, the solution can change rapidly in a short distance and hence complex numerical schemes need to be employed [69].

Young and White [21] were the first to perform 2-D simulations for a condensing steam flow. They were able to show the periodic quenching effect of the nucleation rate on droplet

size distribution. The Eulerian-Eulerian model has been used by several investigators, among which Jan Halama [22], Stastny and Sejna [23], Gerber and Kermani [24], Marcus, F. Bakhtar and K. Zidi [25] and Wlodzimierz and Dykas [26] are the most notables ones. Jan Halama performed 2-D simulations in the supersonic Barschdroff nozzle for an inviscid case using complete Eulerian approach. Another important investigation was done recently by Gerber and Kermani [24] using Eulerian multiphase equations for both vapor and the liquid phase. In this work, concept of classical nucleation theory and droplet interfacial area density for modeling the non-equilibrium condensation in transonic steam flow is utilized. The implicit time integration solution strategy was applied with no constraints on the time-step.

### 3.2 Assumptions of the Model

As discussed earlier, while expanding through a nozzle, steam achieves a supercooled state and then, depending on the degree of supercooling or supersaturation of the vapor, nucleation sets in. Depending on the thermodynamic conditions, the droplets formed from nucleation may grow or evaporate. Since steam (vapor) is a compressible fluid, the governing equations for compressible gas dynamics apply. The numerical algorithm of such compressible flows should take into account the real gas phenomena (using real gas equation of state), owing to the fact that condensing steam deviates from ideal gas behavior. Here, while solving the governing equations for compressible flows it is also important to include the equations for phase transition in condensing flows. The flow governing equations are formulated for the vapor-liquid mixture, i.e., the steam is assumed to be a homogeneous mixture of vapor and mono-dispersed spherical droplets of liquid. This way of formulating a model in terms of the flowing mixture is termed as a single fluid model. Here, some assumptions are made to simplify the model and focus only on the phenomena of nucleation and droplet growth that we are interested in. For simplicity it was assumed that both the phases are governed by the same average pressure P. Furthermore, it is assumed that the volume occupied by the liquid phase is negligible. This gives the following simplified relation between mixture and the vapor density using the wetness fraction

$$\rho = \frac{\rho_v}{1-y},\tag{3.1}$$

where  $\rho$  is the density of the mixture,  $\rho_v$  is the density of the vapor and y is the wetness fraction. The first step is solving the Euler equations governing the condensing flow. It is assumed that the slip velocity between the droplets and vapor is negligible. This lead to the fact that the flow is characterized by a single velocity u for both phases (no-slip condition). This assumption further simplifies the model giving to a single momentum equation. In lowpressure steam, the distance between the liquid droplets is sufficiently large to neglect the interaction between the droplets without loss in accuracy.

### 3.3 Governing Equations

The Laval nozzles considered in the present work have supersonic flow regime i.e. Mach number>1. It is known for steam to behave as compressible flow owing to the fact that they have a Mach number>0.3. Hence it is mandatory to account for compressibility effects in

the governing flow equations for mass, momentum and energy. In this section attention is paid to the governing equations of the compressible flow implemented in the present in-house CFD code. The code is based on time dependent quasi 1-D Euler equations formulated for the vapor-liquid mixture that are coupled with the two additional equations for the nucleation and growth of the liquid droplets. As stated earlier the present model is based on the assumption of mechanical equilibrium condition (i.e., no slip between the vapor phase and the liquid droplets) is satisfied everywhere in the flow field. The assumptions stated in section 3.2 when implemented in the governing equations results in a set of three transport equations for mass, momentum and energy along with two transport equation for liquid phase.

Euler Equations for Mass, Momentum and Energy

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = -\frac{\rho u}{A(x)} \frac{dA}{dx},\tag{3.2}$$

$$\frac{\partial\rho u}{\partial t} + \frac{\partial(\rho u^2 + P)}{\partial x} = -\frac{\rho u^2}{A(x)}\frac{dA}{dx},$$
(3.3)

$$\frac{\partial \rho E}{\partial t} + \frac{\partial ((\rho E + P))u}{\partial x} = -\frac{(\rho u E + Pu)}{A(x)} \frac{dA}{dx},$$
(3.4)

where P is the mixture pressure,  $\rho$  mixture density, u the mixture velocity, E the mixture total specific internal energy.

The change of phase from vapor to liquid do not appear explicitly in the equations (3.2-3.4), but is included in the mixture thermodynamic properties.

It was decided to use in present work the mono-dispersed model. This implies that droplets are assumed to have the same mean radius and thus the size distribution is neglected [55]. Two equations are additionally used, mass conservation of liquid phase y and conservation of droplet number N, to model the non-equilibrium condensation.

Conservation equation for Liquid Phase

$$\frac{\partial \rho y}{\partial t} + \frac{\partial \rho u y}{\partial x} = \Gamma_1 + \Gamma_2, \qquad (3.5)$$

$$\frac{\partial \rho N}{\partial t} + \frac{\partial \rho u N}{\partial x} = J, \qquad (3.6)$$

In equation (3.6), J is the nucleation rate given by the classical nucleation theory and is expressed by equation (2.18). In equation (3.5),  $\Gamma_1$  and  $\Gamma_2$  are the interfacial exchange terms defined as

$$\Gamma_1 = \frac{4}{3}\pi\rho_l r^{*3}J,\tag{3.7}$$

$$\Gamma_2 = 4\pi \rho_l r^2 \frac{dr}{dt},\tag{3.8}$$

where,  $\frac{dr}{dt}$  is the growth rate that is defined by equation (2.28) or (2.30).

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Here  $\Gamma_1$  is the source term of the critical droplets created due to the nucleation process and  $\Gamma_2$  is the mass condensation rate of all the droplets per unit volume of the two-phase mixture  $[kg/(m^3s)]$  for homogeneous condensation.

Equation (3.5) represents the expression for mass conservation for the liquid droplets y whereas equation (3.6) represents the expression for the conservation of the number of droplets N. It can be seen that there is no source term due to condensation in the Euler equations (3.2-3.4), which is attributed to the fact that the gas and liquid phase are summed to give a two-phase homogeneous single pressure model [37].

The following properties are averaged using the mass fraction y, to link the liquid phase properties to that of the vapor phase properties

$$E_m = (1 - y)E_v + yE_l, (3.9)$$

$$h_m = (1 - y)h_v + yh_l. (3.10)$$

$$sos_m = (1 - y)sos_v + ysos_l. ag{3.11}$$

### 3.4 Thermodynamic Model

In order to model the non-equilibrium thermodynamics associated with condensation phenomena, it is essential to take into account the real gas behavior of the steam. In this section attention is given to the choice of the equation of state that can compute the thermodynamic properties in the subcooled region accurately. It is known that the superheated and subcooled steam deviates from the perfect gas behavior, so the calorically perfect ideal gas model does not apply. As seen from the previous section, condensation model, i.e., the nucleation rate and droplet growth is very sensitive to the thermodynamic properties like temperature (supercooling) or pressure (supersaturation). The ideal gas model cannot accurately calculate thermodynamic properties from the values obtained from the solution of the fluid dynamic equations. It is worth noting that it is impossible to describe the state of the mixture using a simple thermodynamic relation such as an equation of state. It was indicated by Callen [30] that the thermodynamic properties in a mixture are defined and have physical meaning only when the condition of local equilibrium is satisfied everywhere in the flow field.

A distinction between the real gases and the ideal gases can be made on account of the intermolecular forces. In the real gases, the intermolecular forces are important while for the ideal gases these forces are negligible. Figure 3.1 shows different thermodynamic conditions which defines the behavior of the gases in pressure-temperature diagram.

It is important to understand the relaxation gas dynamics associated with non-equilibrium condensation process. Relaxation processes can be collectively defined as the way in which gas phase chemical reactions and the excitation of internal modes of molecular energy storage occurs [57]. At the onset of homogeneous nucleation, the system changes to a two-phase system of vapor and liquid. In this scenario, the thermodynamic equilibrium is not attained until the droplet growth process is active, hence there will be exchange of mass, momentum

and energy between the two phases. In order to have a physical understanding of the complex flow field, it is important to understand the role of the relaxation time associated with each process in bringing the system back to equilibrium. The guidelines for three relaxation times suggested by Guha and Young [56] are adopted, i.e., thermal equilibrium of the droplets, interface slip velocity and the thermal equilibrium of the complete system. It is suggested that the droplets, formed on the onset of the homogeneous nucleation process, try to reach the thermodynamic equilibrium, i.e., its equilibrium temperature in the shortest time. Hence the relaxation time associated with thermal equilibrium of the droplets is the smallest. On this theory, the droplet temperature can be approximated to be equal to that of the saturation temperature  $T_s(\mathbf{P})$  without loss in accuracy of the model. The assumption of no-slip condition is based on the second relaxation time associated with momentum transfer process, which is quick when the droplet size is very small ( $r \ll 10^{-6}$  m). Under this assumption it can be stated that the interface of the momentum transfer reaches the equilibrium value fast, hence there is no velocity difference between the liquid and the vapor phase. Lastly the third relaxation time is associated with process of the vapor temperature reaching its equilibrium value that eventually brings the whole system of mixture flow to equilibrium condition. This process is relatively slower and hence is considered as frozen in time. It can now be deduced that the mechanism of the liquid and vapor phase is uncoupled. As the variations driven by flow field is much faster than thermal variation due to condensation and hence gas phase flows like a single phase vapor [37].



Figure 3.1: Different gas region on a P-T Diagram [1].

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#### 3.4.1 Non-Equilibrium Equation of State: Wet Steam

A comprehensive literature is available on the various types of equations of state for computing thermodynamic properties of steam. However, the most accurate and recommended equation of state for steam for industrial applications is the "IAPWS Industrial Formulation 1997" (IAPWS-IF97). The International Association for the Properties of Water and Steam (IAPWS) Industrial Formulation 1997 consists of a set of equations for different regions. The basic equation for each region is based on fundamental expression for specific Gibbs free energy. However, in the in-house CFD code in order to estimate the thermophysical properties and their partial derivatives, a common interface to several thermodynamic models (Fluid-Prop) has been used [59] [60]. The thermodynamic library computes the fluid thermodynamic and transport properties. It was chosen to use cubic form of Equation of State (EoS), derived from Peng Robinson equation. It estimates the thermodynamic state in the metastable region accurately and hence leads to accurate prediction of the condensation model. The cubic EoS makes the solution of the flow equations faster as compared to the Multi-parameter Equation of State (MEoS) due to its simple form. Complete details of the used cubic EoS is given by Colonna [61]. Here a brief explanation is introduced for the sake of completeness. The PRSV (Peng-Robinson-Stryjek-Vera) EoS is similar to the cubic form proposed by Peng and Robinson [58]

$$P = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2},\tag{3.12}$$

where

$$a = \left(\frac{0.457235R^2T_c^2}{P_c}\right)\alpha,\tag{3.13}$$

$$b = \left(\frac{0.077796RT_c}{P_c}\right),\tag{3.14}$$

and

$$\alpha = \left[1 + \kappa \left(1 - \sqrt{T_r}\right)\right]^2. \tag{3.15}$$

The modification introduced by Stryjek and Vera [62], makes  $\kappa$  temperature-dependent

$$\kappa = \kappa_0 + \kappa_1 \left( 1 + \sqrt{T_r} \right) (0.7 - T_r), \qquad (3.16)$$

with,

$$\kappa = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3.$$
(3.17)

The improved PRSV EoS, iPRSV is obtained by modifying the equation for the calculation of  $\kappa$  value, such that it is continuous with the temperature, but by keeping the same parameters  $\kappa_0$  and  $\kappa_1$  in the functional form, with same values. The  $\kappa$ - function in the iPRSV thermodynamic model is therefore

$$\kappa = \kappa_0 + \kappa_1 \left\{ \sqrt{\left[A - D\left(T_r + B\right)\right]^2 + E} + A - D\left(T_r + B\right) \right\} \sqrt{T_r + C}.$$
 (3.18)

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The thermodynamic properties of the vapor phase are calculated based on the iPRSV equation of state. The iPRSV formulation can be used for calculating thermodynamic properties of the droplets at low pressures.

### 3.5 Numerical Methods

The Euler equations are hyperbolic partial differential equations. The hyperbolic systems of partial differential equations (Euler equations) can be used to model a wide variety of phenomena that involve wave motion. A general form of the equation of motion, is given by equation (3.19) for arbitrary EoS and is restricted to the quasi 1-Dimensional Euler equations

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0, \qquad (3.19)$$

here Q and F constitutes the vector of the conservative variables and the flux vector respectively, given as

$$Q = \begin{bmatrix} \rho \\ m \\ E \end{bmatrix}, \tag{3.20}$$

$$F = \begin{bmatrix} m \\ \frac{m^2}{\rho} \\ (E+P)\frac{m}{\rho} \end{bmatrix}, \qquad (3.21)$$

where  $m = \rho u$ , is the momentum per unit volume, u is the mixture velocity, and E is the mixture specific total internal energy per unit volume and can be expressed as

$$E = h_m - \frac{P}{\rho_m} + \frac{1}{2}u \cdot u. \tag{3.22}$$

In this section only a brief overview of the numerical scheme is presented, however for detailed numerical schemes book by Randall J. Leveque [63] can be referred. In the present work finite volume method is used, which is derived from the integral form of the conservation laws as given by equation (3.23). The finite volume method mimics the conservation laws by conserving the quantities like mass, momentum and energy irrespective of the size of computational domain. This method is based on segmenting the spatial domain under consideration into a number of intervals, termed as finite volumes or grid cells. An approximation to the integral of the conserved quantity q is done over each of these control volumes. This is followed by updating these values through approximations of the flux through the endpoints of the interval. The primary problem is to determine good numerical flux functions that approximate the correct fluxes reasonably well, based on the approximate cell averages.

$$\frac{d}{dt} \int_{C_i} q\left(x,t\right) dx = f\left(q\left(x_{i-\frac{1}{2}},t\right)\right) - f\left(q\left(x_{i+\frac{1}{2}},t\right)\right), \qquad (3.23)$$

and  $i^{th}$  grid cell is represented by

$$C_{i} = \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right), \qquad (3.24)$$

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where  $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$  is the length of the cell. We can use the expression given by equation (3.23) to develop an explicit time-marching algorithm. If we are given a quantity at time  $t_n$ , then we can approximate the quantity at the next time level  $t_{n+1}$  after a step length of  $\Delta t = t_{n+1} - t_n$ . Integrating equation (3.23) from time  $t_{n+1}$  to  $t_n$  will yield

$$\int_{C_{i}} q(x, t_{n+1}) dx - \int_{C_{i}} q(x, t_{n}) dx = \int_{t_{n}}^{t_{n+1}} f\left(q\left(x_{i-\frac{1}{2}}, t\right)\right) dt - \int_{t_{n}}^{t_{n+1}} f\left(q\left(x_{i+\frac{1}{2}}, t\right)\right) dt.$$
(3.25)

Rearranging equation (3.25) and dividing by  $\Delta x$  gives

$$\frac{1}{\Delta x} \int_{C_i} q(x, t_{n+1}) \, dx = \frac{1}{\Delta x} \int_{C_i} q(x, t_n) \, dx - \frac{1}{\Delta x} \left[ \int_{t_n}^{t_{n+1}} f\left(q\left(x_{i-\frac{1}{2}}, t\right)\right) \, dt - \int_{t_n}^{t_{n+1}} f\left(q\left(x_{i+\frac{1}{2}}, t\right)\right) \, dt \right].$$
(3.26)

The above equation imparts the fact how the cell average of quantity q should be updated in one time step. Let us say the value Q, is the approximate average value over the  $i^{th}$  interval at time  $t_n$ , then we have

$$Q_{i}^{n} \approx \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x,t_{n}) dx \equiv \frac{1}{\Delta x} \int_{C_{i}} q(x,t_{n}) dx.$$
(3.27)

Substituting equation (3.27) in equation (3.26) we have

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( F_{i+\frac{1}{2}}^n - F_{i-\frac{1}{2}}^n \right), \qquad (3.28)$$

where  $F_{i\pm\frac{1}{2}}^n$  is an approximation of the average flux along  $x=x_{i\pm\frac{1}{2}}$  and is given by

$$F_{i-\frac{1}{2}}^{n} \approx \frac{1}{\Delta t} \int_{t_{n}}^{t_{n+1}} f\left(q\left(x_{i-\frac{1}{2}}, t\right)\right) dt.$$
(3.29)

It is well understood that in a hyperbolic problem information propagates with finite speed, so it is reasonable to first suppose that we can obtain  $F_{i-\frac{1}{2}}^n$  based only on the values  $Q_{i-1}^n$  and  $Q_i^n$ , the cell averages on either side of this interface. Giving the flux a new formulation

$$F_{i-\frac{1}{2}}^{n} = \mathcal{F}\left(Q_{i-1}^{n}, Q_{i}^{n}\right), \qquad (3.30)$$

where  $\mathcal{F}$  is a numerical flux function. Thus, equation (3.28) becomes

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( \mathcal{F} \left( Q_i^n, Q_{i+1}^n \right) - \mathcal{F} \left( Q_{i-1}^n, Q_i^n \right) \right).$$
(3.31)

Equation (3.31) is the final expression for the calculation of the conserved quantity Q ( $\rho$ ,  $\rho u$ ,  $\rho E$ ) at next time level and it strongly depends on the specific method chosen to calculate  $\mathcal{F}$ , the numerical flux at the interface.

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**Figure 3.2:** Illustration of a finite volume method for updating the cell average  $Q_i^n$  by fluxes at the cell edges. Shown in x-t space [63].

There are generally two families of techniques for discretizing the time derivatives: explicit and implicit methods. In an explicit method, the unknown variables at a given time step are obtained from the information of variables from previous time steps only. Implicit methods, on the other hand, simultaneously advances every grid point, and are therefore more complex than their explicit counterparts. Implicit techniques involve more computation per time step, because of the large matrix inversions involved. A Forward-Euler method is implemented in the code with Courant-Friedrichs-Lewy (CFL) numbers below 1 were used. The CFL condition must be satisfied, while solving certain partial differential equations, by any finite volume or finite difference method if we expect it to be stable and converge. The time step must be less than a certain time in many explicit time-marching simulations, otherwise the simulation will produce incorrect results [63]. This implies that the information must propagate at the correct physical speeds. The CFL number is expressed by equation (3.32) in one dimensional form

$$C = \frac{u \,\triangle t}{\Delta x},\tag{3.32}$$

where u is the magnitude of velocity,  $\Delta t$  is the time step and  $\Delta x$  is the length of the interval. The applied method in the present work is an explicit method meaning that the value  $Q^{n+1}$  will depend on the value of  $Q^n$ .

#### 3.5.1 Convective Fluxes

The convective fluxes are calculated at the cell interfaces by solving the Riemann problem between two neighboring cells. It was Godunov [65] who proposed the solution for the local Riemann problem and it is based on the exact solution of the one-dimensional Riemann problem. In the one-dimensional case, Godunov scheme fulfills the positivity of density and pressure for the Euler system. However it has several drawbacks like it is only first order and is computationally expensive for solving exact Riemann Problem. These problems gave way for the development of Approximate Riemann Solvers (ARS). The most commonly used schemes are Roe's linearization [66] and the Advection Upstream Splitting Method (AUSM) by Liou [4]. A major drawback associated with Roe's linearisation is the failure in fulfilment of the entropy condition and has to be enforced.

AUSM<sup>+</sup> scheme, which is implemented in present code, is discussed briefly. AUSM<sup>+</sup> formulated by Liou has some interesting features such as:

- Exact resolution of 1D contact and shock discontinuity,
- positivity-preserving of scalar quantity such as density,
- simplicity of the algorithm,
- free of oscillations at the slowly moving shock,
- easy extension to treat other hyperbolic systems.

The AUSM<sup>+</sup> scheme is an improved version of AUSM scheme. In the AUSM scheme by Liou [70], the Euler fluxes are split into convective and acoustic waves and are considered as two distinct processes:

$$\mathbf{F}^{n}(\mathbf{Q}(x,t)) = \mathbf{F}^{n} + \mathbf{P} = \mathbf{M} \begin{pmatrix} \rho \\ m \\ \rho h_{t} \end{pmatrix} + P \begin{pmatrix} 0 \\ \mathbf{n} \\ 0 \end{pmatrix}, \qquad (3.33)$$

where  $h_t$  is the total enthalpy.

Here the convective flux  $\mathbf{F}^{(n)}$  is expressed in terms of convective speed M and passive scalar quantities. The pressure flux  $\mathbf{P}$  contains only the pressure term.

Thus the numerical flux  $\mathbf{F}_{(i+\frac{1}{2})}^n$  at the interface is defined as the sum of the numerical convective flux  $\mathbf{F}_{(i+\frac{1}{2})}^n$  and the numerical pressure flux  $\mathbf{P}_{i+\frac{1}{2}}$  at the interface  $i + \frac{1}{2}$ :

$$\mathbf{F}_{(i+\frac{1}{2})}^{n} = \mathbf{F}_{(i+\frac{1}{2})}^{(c)} + \mathbf{P}_{i+\frac{1}{2}} = \mathbf{M}_{i+\frac{1}{2}} \ c_{i+\frac{1}{2}} \ \Psi_{i+\frac{1}{2}} + p_{i+\frac{1}{2}} \begin{pmatrix} 0 \\ \mathbf{n} \\ 0 \end{pmatrix},$$
(3.34)

where  $\Psi = (\rho, m, \rho h_t)^T$ , and is defined in the interface as:

$$\Psi_{i+\frac{1}{2}} = \begin{cases} \Psi_i, & \text{if } \mathcal{M}_{i+\frac{1}{2}} \ge 0, \\ \Psi_{i+1}, & \text{otherwise.} \end{cases}$$
(3.35)

In the new AUSM<sup>+</sup> scheme a common speed of sound  $c_{i+\frac{1}{2}} = c(\mathbf{Q}_{i+1}, \mathbf{Q}_i)$  is defined at the cell interface resulting in unification of the Mach number and velocity. This unification allows in exact capturing of a shock wave. Finally, the flux expression given by the AUSM<sup>+</sup> method can be written as:

$$\mathbf{F}_{(i+\frac{1}{2})}^{(c)} = \frac{1}{2} c_{i+\frac{1}{2}} \left[ m_{i+\frac{1}{2}} (\Psi_i + \Psi_{i+1}) - |m_{i+\frac{1}{2}}| (\Psi_i - \Psi_{i+1}) \right] + p_{i+\frac{1}{2}} \begin{pmatrix} 0\\ \mathbf{n}\\ 0 \end{pmatrix}.$$
(3.36)

where the interface quantities are defined as:  $m_{i+\frac{1}{2}} = \mathfrak{M}_i^+ + \mathfrak{M}_{i+1}^-$  and  $p_{i+\frac{1}{2}} = \mathfrak{P}_i^+ p_i + \mathfrak{P}_{i+1}^- p_{i+1}$ . The unknown variables are estimated as:

$$\mathfrak{M}^{\pm}(\mathbf{M}) = \begin{cases} \frac{1}{2} \left(\mathbf{M} \pm |\mathbf{M}|\right), & \text{if } |\mathbf{M}| \ge 1, \\ \pm \frac{1}{4} \left(\mathbf{M} \pm 1\right)^2 \left(2 + 4\beta \left(\mathbf{M} \mp |\mathbf{M}|\right)^2\right), & \text{otherwise.} \end{cases}$$
(3.37)

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and

$$\mathfrak{P}^{\pm}(\mathbf{M}) = \begin{cases} \frac{1}{2} (1 \pm |\mathbf{M}|/\mathbf{M}), & \text{if } |\mathbf{M}| \ge 1, \\ \frac{1}{4} (\mathbf{M} \pm 1)^2 \left( 2 \mp \mathbf{M} \mp 4\alpha \mathbf{M} (\mathbf{M} \mp |\mathbf{M}|)^2 \right), & \text{otherwise.} \end{cases}$$
(3.38)

with  $\alpha = \frac{3}{16}$  and  $\beta = \frac{1}{8}$  as the original paper [4].

Liou's scheme automatically enforces the entropy condition and positively preserves scalar quantities (like for example density) [4].

### 3.6 Implementation Strategy for Condensation Model

In this section the methodology used to implement the condensation model in the existing CFD code is discussed.

A time marching scheme is being implemented in the code whereby the conservative flow field of the next time step will be updated using information of the conservative flow field from previous time level. The thermodynamic library is used to update the thermodynamic states after every time step. The density and the internal energy are chosen as the independent thermodynamic variables since they are updated at the end of each time step in the Eulerian solver. The pressure P of the mixture is then calculated using the relation for the total energy of the mixture E given by

$$E - h_v(1 - y) - h_l y + \frac{P}{\rho} - \frac{1}{2}u^2 = 0$$
(3.39)

The applied EoS for the vapor and the liquid is non-linear which results in a non-linear relation for pressure. Thus, the equation (3.39) is solved by means of the Newton iteration scheme. As discussed earlier, the density of vapor is calculated using equation (3.1). Now knowing the pressure and density of the vapor other variables such as the speed of sound c, isentropic coefficient  $\gamma$ , enthalpy h, entropy s, saturation temperature  $T_s$  and saturation pressure  $P_s$ , etc. can be calculated using thermodynamic library. Similarly the liquid phase variables are calculated using pressure P of the mixture and saturation temperature  $T_s$  as independent variables. Followed by this, the source terms resulting from condensation are calculated, i.e., the nucleation and growth of the droplets. The conditions used for the onset of the nucleation and the droplet growth are depicted in figure 3.3.

The first case in the figure 3.3 implies if the supersaturated vapor has droplets of radius less than or equal to the critical radius, there is only nucleation and no growth of the droplets.



Figure 3.3: Conditions for the onset of Nucleation and the Droplet Growth.

Whereas the second case implies that if both the conditions of supersaturated vapor and the radius of the droplets exceeding the critical radius are satisfied, then there is nucleation of droplets and further growth of the already nucleated droplets. The process of nucleation and the droplet growth contributes to the source term on the right hand side of the conservation equations (3.5 and 3.6) for liquid phase.

The figure 3.4 shows a flow diagram that outlines the methodology implemented in the present code. It can be seen from the flow diagram that the numerical domain, the boundary conditions and the thermodynamic library are specified as input to the CFD code. Then the flow field is initialized using the boundary conditions and assigning the values to the conservative variables in each control volume. The initial conditions are then known using these conservative variables. The next step is to calculate the time step using the CFL condition. To calculate the convective fluxes the AUSM<sup>+</sup> scheme [4] is used as discussed earlier. It is now possible to calculate the flux balance knowing the flux differences and other source terms like the derivative of area of nozzle and the source terms of condensation model. Now the solution is advanced in time by updating the conservative variables from the information of the variables at the previous time level. From these updated conserved variables, the new thermodynamic state of the system consequently the source terms are calculated. The methodology will be repeated according to the predefined maximum iterations until a converged solution is reached.



Figure 3.4: Flow diagram of the implemented Euler equations solver in steady mode.

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## Chapter 4

## **Results and Discussion**

The objective of this chapter is to validate the implemented condensation model described in the chapter 2. In order to assess the accuracy, experimental data of various 1-D supersonic nozzle is compared to the results obtained by present model.

## 4.1 Overview of the Validation Process

The condensation model is validated in the present work by a number of quasi 1-D flow in supersonic nozzles of different geometries. The reason behind selecting nozzle test cases is the fact that they form a benchmark for testing the condensation models. The convective behavior of supersonic steam flow found in low-pressure steam turbines with condensation, is essentially incorporated in the solution of the quasi 1-D Euler equations [1]. Thus, the solutions find their practical applications in the steam turbines. The accuracy of any condensation model relies on the quality of the underlying nucleation and the droplet growth theory. These theories can be tested for their accuracy if the experimental data for the pressure distribution and the droplets size are available. In order to validate the condensation model, the pressure distribution of the flow and the droplet growth theory needs to be tested for its accuracy and reliability in predicting the size of the droplets. Followed by this the nucleation theory is tested for its accuracy, given the uncertainties in this theory. As discussed earlier, the surface tension of the spherical droplets play a vital role in determining the accuracy of the nucleation theory.

There is a comprehensive amount of literature and well documented experimental data available on spontaneous condensation in the transonic and supersonic nozzles. In the light of the approach outlined above, these data are collected and used for validation of the implemented condensation model. In the sections to follow the results and analysis of simulations carried out in various 1-D supersonic nozzles will be presented.

### 4.2 Supersonic Condensing Nozzle Tests

### 4.2.1 Barschdorff's Nozzle

The Barschdorff's experiment [67] on a supersonic nozzle is the first test case selected for validation. The nozzle used by Barschdorff in his experiment is an arc Laval nozzle, with the radius of the wall curvature of 584 mm and the critical throat height of 60 mm. The geometry of the nozzle is shown in figure 4.1. Two test cases were considered with two different boundary conditions that correspond to those in the Barschdorff's experiment. The first case implements the boundary conditions, i.e., the total pressure at the inlet of  $P_0=78,390$  Pa and the total temperature at the inlet of  $T_0=380.55$  K, while the second case is with the same total pressure but with lower total temperature at the inlet of  $T_0=373.17$  K. The outlet from the nozzle is supersonic for both the test cases so Neumann conditions are applied.

Figures (4.2-4.4) depict the results of the first test case simulation, i.e., the main flow parameters which are important in the steam flow with spontaneous condensation. Figure 4.2a shows the static pressure distribution along the nozzle axis and is compared with experimental result. It can be observed that at the nozzle position of approximately x=0.05 the pressure jump called the condensation shock starts and is well captured by the present numerical model. The pressure jump in the flow is a result of the heat released by the condensation process, which tends to slow down the flow. The drop in velocity of the flow can be observed from the decrease in Mach number as shown in figure 4.2b. The heat released is sub-critical heat, which implies that flow remains supersonic in spite of the condensation shock. This phenomena results in a higher static pressure at the exit of the nozzle as compared to the dry steam flow. The steam at the inlet of the nozzle is dry and superheated, which can be deduced from the fact that supersaturation ratio S is well below 1 as seen in figure 4.2c. As the steam expands through the nozzle, the supersaturation ratio S increases and attains the value of unity. At this point the saturation line of the vapor phase is crossed. As expected the nucleation is not triggered as soon as the saturation line is crossed, but is delayed until the supersaturation ratio becomes high enough to reduce the critical radius  $r^*$ . The reduction in critical radius  $r^*$  results in the formation of the discernible amount of droplets and



Figure 4.1: Barschdorff Nozzle [68].

hence nucleation is triggered. This nucleation of the droplets is seen in the form of nucleation rate J shown in figure 4.3a. It can be seen from figure 4.2c, S continues to rise until the spontaneous condensation occurs. The heat released as a result of the condensation process tends to decrease the supersaturation and hence the nucleation rate. This can be observed in figure 4.2c and 4.3a. The release of latent heat of condensation prevents further subcooling of the steam and hence subcooling level drops as seen in figure 4.4a. However the wetness of the steam continues to increase as shown in figure 4.3d, owing to the fact that the flow has entered the condensation region as the droplet growth rises [69]. The growth of the droplets occurs as a result of the condensation on the droplets formed during the nucleation process, increasing the size of the droplets and hence increasing the liquid mass fraction. However, the number of droplets remains the same and there are no new droplets formed after the spontaneous condensation has occurred. Thus, it can be said that the nucleation supplies the droplet number and the droplet growth supplies the liquid mass fraction. The dependence of the nucleation rate on the supersaturation can be observed from the fact that both have their peaks at the same location in the nozzle. From figure 4.2d, it can be observed that the temperature of the vapor rises at approximately x=0.05, as a result of nucleation, and hence the vapor temperature at the exit of the nozzle is higher as compared to the isentropic flow. From the results shown it can be observed that the subcooling precedes the nucleation. Also the wetness fraction of the flow is significant only after the peak of nucleation is reached and the vapor temperature reaches its equilibrium value. The figure 4.4b shows that the process is indeed an irreversible process and hence there is change in entropy.

Figures (4.5-4.7) depict the results of the second test case simulation. It can be observed from these figures that the presented model predicts similar condensation phenomena as described earlier for the first test case. In the second test case with a lower total inlet temperature, due to lower expansion rate, the condensation shock appears more upstream as compared to the first test case.

The condensation model, i.e., the nucleation rate and droplet growth rate, implemented in the present work is compared with the one implemented by Dykas [26]. Dykas had used a single fluid model to simulate the flow in Barschdorff's nozzle with the same two test cases presented here in this work. It can be deduced from figure 4.3 that the implemented nucleation and growth theories are in close agreement with that implemented by Dykas. It is to be pointed out here that in the model presented by Dykas, the EoS recommended by IAPWS was used, while we have used the IPRSV cubic EoS discussed earlier. This justifies the deviation of thermodynamic states like the temperature of vapor (fig 4.2d) predicted by the equation of state in the present model from that of Dykas model. Also the droplet radius predicted by Dykas model for the first test case was almost 40 % lower than that observed by Barschdorff during experiments (droplet radius predicted by Barschdorff r=6.67E-08m). While the model in the present work predicts the droplet radius very close to that of Barschdorff's experimental value. The droplet radius computed by present model is in reasonable agreement with the experimental results considering the uncertainty in the measurement of droplet size at this scale.

It can be deduced from the results of the simulations for the two test cases of Barschdorff's nozzle that the boundary conditions imposed play a key role in the location of the condensation shock in the nozzle. It can be observed from the two test cases of the Barschdorff's nozzle that condensation onset is delayed by increasing the inflow stagnation temperature. The more upstream the location of spontaneous condensation point in the nozzle is, the larger is the

sudden pressure rise at the nozzle centerline. This can be observed from the second test case of the Barschdorff's nozzle experiment. Otherwise this sudden pressure rise is smaller as in the first test case of the Barschdorff's nozzle experiment. Also it can be observed from the two test cases that more the downstream condensation onset is, larger is the subcooling level



**Figure 4.2:** Barschdorff's Nozzle first test case: (a) Pressure, (b) Mach number, (c) Supersaturation ratio and (d) Vapor temperature distribution along the nozzle axis.

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**Figure 4.3:** Barschdorff's Nozzle first test case: (a) Nucleation rate, (b) Number of Droplets, (c) Droplet radius, (d) Wetness fraction distribution along the nozzle axis.

and larger is the number of droplets formed.

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**Figure 4.4:** Barschdorff's Nozzle first test case: (a) Subcooling level, (b)Entropy distribution along the nozzle axis.

#### 4.2.2 Moore's Nozzle

For this test case experimental data from Moore et al. [20] was used. The geometry of the converging-diverging nozzle is shown in the figure 4.8 and it is the one used by Moore in his experiment. The boundary conditions at the inlet of the nozzle were taken to be same as that of Moore et al. experiment, i.e., total pressure at the inlet of  $P_0 = 25$  KPa and the total temperature at the inlet of  $T_0 = 356.6$  K. The outlet from the nozzle is supersonic, therefore Neumann conditions are applied. Figures (4.9-4.10) depict the results of the computations performed by the implemented condensation model and is compared with condensation model implemented by Yang and Shen [73]. It can be observed from these figures that the implemented model is able to compute the expected traits of the spontaneous condensation process in a supersonic nozzle. As discussed earlier owing to the lower total temperature and pressure at the inlet of the nozzle the location of the onset of condensation is shifted further upstream of the nozzle as compared to the Barschdorff's nozzle. Again it can be observed from the figure 4.9a that the present model is able to capture the static pressure distribution along the nozzle axis with reasonable accuracy when compared with experimental results. Also the heat released due to condensation is sub-critical. This implies that the flow remains supersonic in spite of the appearance of the condensation as shown in the figure 4.9b.

#### 4.2.3 Discussion

The results presented in the previous section show that the condensation model implemented is able to predict the location of condensation shock and hence the pressure rise within reasonable accuracy. Also the droplet radius computed by the presented model is in close agreement with the experimental value given the uncertainty of the measurement of droplet



**Figure 4.5:** Barschdorff's Nozzle second test case: (a) Pressure, (b) Mach number, (c) Supersaturation ratio and (d) Vapor temperature distribution along the nozzle axis.

size at this scale. However, it is discussed here how the assumptions made in the model influence the results obtained.

The single fluid model implemented in the present work assumes no slip velocity between the two phases. In contrast to this the two fluid model predicts the slip velocity between the two phases and hence shows the correct behavior of the applied drag forces [26]. It is essential to take into account drag forces in the momentum equation for a correct prediction of the velocity field. Also as observed by Dykas [26], the two fluid model is able to predict the droplet radius quite accurately as compared to single fluid model.



**Figure 4.6:** Barschdorff's Nozzle second test case: (a) Nucleation rate, (b) Number of Droplets, (c) Droplet radius, (d) Wetness fraction distribution along the nozzle axis.

In the presented model the droplet temperature was assumed to be equal to the saturation temperature  $T_s(P)$ . However, it is possible to determine the temperature of the droplets by the capillarity effect using the expression (4.1) given by Gyarmathy [12] and since the droplets formed during condensation are very small in size their temperatures can be assumed to be uniform inside the droplet

$$T_{droplet} = T_s(P) - [T_s(P) - T_v] \frac{r^*}{r},$$
(4.1)

where  $T_{droplet}$  is the temperature of the droplet. The above expression relates the temperature of the droplet to its size. It is proposed to include the temperature of the droplet in the growth

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Figure 4.7: Barschdorff's Nozzle second test case: (a) Subcooling level, (b) Entropy distribution along the nozzle axis.



Figure 4.8: Geometry of the supersonic nozzle used by Moore et al. [73].

rate equation in the future and analyze its effects in predicting the droplet size.

As discussed earlier the interaction between the liquid droplets has been neglected in the present work. However, the droplet size distribution may vary as droplets may collide with each other and stick together. This mechanism can be tested using an agglomeration rate expression and typical mean droplet radius. Moses and Stein [71] observed very small agglomeration rates during their experimental work on supersonic nozzles. This feature allows to study the growth of the droplets in the supersonic nozzles without dealing with complicated stochastic agglomeration phenomena.



**Figure 4.9:** Moore's Nozzle test case: (a) Pressure, (b) Mach number, (c) Supersaturation ratio and (d) Vapor temperature distribution along the nozzle axis.

White [72] investigated the viscous effects on condensation process. In the present work an inviscid flow is assumed in the supersonic nozzle to study condensation. However, White's studies suggest that boundary layer effects are likely to influence the condensation process in two major ways. First, the fluid particles passing through the boundary layer travel slowly than in free stream. This effect results in lower expansion rates and hence smaller departures from equilibrium. Second, the viscous heat and the conduction of heat from hotter zones may prematurely truncate the nucleation in boundary layer flow. As a result of these two effects the number of droplets nucleated is reduced, ultimately leading to larger droplet size on establishment of the equilibrium conditions. Thus, the average droplet radii and size



**Figure 4.10:** Moore's Nozzle test case: (a) Nucleation rate, (b) Subcooling Level, (c) Droplet radius, (d) Wetness fraction distribution along the nozzle axis.

distribution predicted by the viscous flow are expected to differ considerably from those predicted by the inviscid flow. Hence, it is proposed to extend the present work to viscous flows and analyze the viscous effects on the condensing flows. 

# Chapter 5

## **Conclusions and Recommendations**

A completely Eulerian model to solve the wet steam flow in supersonic nozzles has been implemented in the present work. In addition to the fluid dynamic equations, two additional equations were implemented into the Euler equations to predict the nucleation and growth of the droplets. Also the numerical techniques involved to solve the Eulerian flow governing equations were discussed. The theoretical background of the homogeneous condensing flow was described. It was observed that the actual transition of phase occurs only after a certain level of homogeneous nucleation has been triggered and droplet growth has stabilized, which ultimately leads to formation of the stable liquid droplets. The latent heat release, which is a characteristic behavior of any condensation process, leads to a complex interaction between the flow field and the condensation processes resulting in a change of the flow pattern. It was also discussed how the accuracy of a condensation model depends on its constitutive elements, i.e., the nucleation and the droplet growth theory. It was seen that knowing the experimental pressure profiles and droplet size data, it is possible to check the accuracy of the theoretical condensation model. The nucleation theory implemented in the present work is based on the assumption of capillarity and is based on the classical nucleation theory. This implies that the macroscopic thermodynamic equilibrium parameters are used to describe a non-equilibrium microscopic process [37].

The accuracy of the condensation model implemented in the CFD code was tested on 1-D Laval nozzles. The results obtained from the simulations showed the expected traits of wet steam flow. The numerical techniques has proved to be robust in solving the flow governing equations in different 1-D nozzles. Finally the comparison with experimental data verified that the implemented model is physically accurate. It was observed from the results that the droplet radius predicted by the implemented model lacks quantitative accuracy when compared with experimental data. This is attributed to the fact that the growth rate equation (2.28) devised by Gyarmathy implemented in the presented work adopts a correction factor, which is too high for the Knudsen number range experienced in the nozzles tested. This leads to an inaccurate prediction of the growth of the droplets. Also, it is very important to accurately evaluate the rate of heat released as it determines the actual axial position at which nucleation is quenched along with droplet number and size of droplets [37]. It is also

seen that the present model is able to predict the location and intensity of condensation shock well.

The present work is a simple and effective step for the development of a condensation model. In order to utilize the present model for engineering applications, the inclusion of viscous and non-adiabatic terms is important. It will be an interesting study to compare the results of the present model with those of the two-fluid model. Also, a check on the dependence of the present model on the type of equation of state should form a part of future studies. For instance the evaluation of the model based on equation of state recommended by IAPWS is suggested. As discussed earlier the value of surface tension of very small droplets influences the results in a major way. It is recommended to assess the effect of surface tension values that include size variation, on the present model.

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## Appendix A

## Evaluation of the Steady State Nucleation Rate

The analytic solution of the equation (2.16) is evaluated by substituting the value of  $n_g$  from equation (2.13) to give

$$J_{CL} = \left[ \int_{g=1}^{\infty} \frac{1}{C_g n_1 exp\left(\frac{-\Delta G}{KT_v}\right)} dg \right]^{-1}.$$
 (A.1)

 $C_g$  is proportional to  $g^{\frac{2}{3}}$  and varies slowly with g (g-mer) as compared to the rapidly changing exponential term in the denominator of equation (A.1). For this reason  $C_g$  is approximated as  $C_{g_*}$ . Now the  $\Delta G$  is expanded using Taylor series expansion about  $g_*$  as

$$\Delta G = \Delta G_* + (g - g_*) \left(\frac{\partial \Delta G}{\partial g}\right)_* + \frac{(g - g_*)^2}{2} \left(\frac{\partial^2 \Delta G}{\partial g^2}\right)_* + \dots \dots$$
(A.2)

Truncating after the second-order term and noting that  $\left(\frac{\partial\Delta G}{\partial g}\right)_* = 0$ , equation (A.1) becomes

$$J_{CL} = C_{g_*} n_1 Z exp\left(\frac{-\Delta G_*}{KT_v}\right),\tag{A.3}$$

where Z is called Zeldovich factor, given by

$$\frac{1}{Z} = \int_{g=1}^{\infty} exp \left[ -\left(\frac{\partial^2 \Delta G}{\partial g^2}\right)_* \frac{\left(g - g_*\right)^2}{2KT_v} \right] dg \cong \left[ \frac{-\left(\frac{\partial^2 \Delta G}{\partial g^2}\right)_*}{2\pi KT_v} \right]^{-\frac{1}{2}}$$
(A.4)

Evaluating  $\left(\frac{\partial^2 \Delta G}{\partial g^2}\right)_*$  from equation (A.5)

$$\frac{\Delta G}{KT_v} = \frac{A\sigma}{KT_v} g^{\frac{2}{3}} - glnS,\tag{A.5}$$

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where K is Boltzmann's constant and  $A = 36\pi \left(\frac{m}{\rho_l}\right)^{\frac{2}{3}}$ .

Substituting the value of  $\left(\frac{\partial^2 \Delta G}{\partial g^2}\right)_*$  into equation (A.3) gives the final expression (2.17) in the main text.