

Article

A CFD Model for the Evaporation of Sub-Micron Droplet Sprays Across Normal Shocks

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Abstract

The rapid evaporation of liquid droplets across a normal shock wave is a phenomenon of critical importance in advanced propulsion and clean energy systems, such as NH₃ supersonic separation. The conventional Spalding d^2 -law is commonly used to model such phenomena, but it is not suitable for predicting the complete vaporization of sub-micron droplets, particularly as evaporation approaches the free-molecular regime. To address this issue, this paper introduces a novel time-dependent one-dimensional CFD model, which is used to analyze the shock structure, the non-equilibrium heat and mass transfer between the liquid and gas phases, and the evolution of the droplets' size through the shock. The model describes the evaporation of NH₃ sub-micron droplet sprays across a stationary normal shock for various fractions of the liquid phase. The Gyarmathy evaporation model is utilized to accurately account for the transition from diffusion-governed to free-molecular regimes, alongside a new two-phase Rankine–Hugoniot shock jump formulation. The study reveals the influence of a steady normal shock on the physical structure of a droplet-laden flow, including the existence of an initial droplet size swelling through the shock, and quantifies the subsequent complete evaporation of the suspended droplets. The maximum swelling throughout the shock is up to 17%, which corresponds to the case with 8% liquid phase mass fraction in the flow. The model provides acceptable accuracy in calculating the two-phase parameters in high-speed flows and can be extended for modeling more complex, multidimensional detonation and propulsion systems.

Keywords: evaporation; spray; droplet; normal shock; detonation

Academic Editor: Rama Subba Reddy Gorla

Received: 19 December 2025

Revised: 26 January 2026

Accepted: 20 February 2026

Published: 25 February 2026

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1. Introduction

Two-phase flows involving dispersed liquid droplets are fundamental to a vast array of cutting-edge energy and propulsion systems. These phenomena are critical across fields ranging from fuel atomization in gas turbines and aeronautical engines to specialized chemical separation processes [1–6]. The overall efficiency and performance of these complex systems, particularly when operating in high-speed regimes, are intricately governed by the dynamics of droplet phase change, specifically condensation and evaporation. Examples of where these processes are vital include supersonic expansion [7–9], spray

compression during shocks [10–13], detonation suppression [14,15], spray drying, and internal combustion engines [1–3,16].

A particularly challenging and scientifically rich scenario involves droplet-laden flows subjected to rapid compression by a normal shock wave [14]. This is a crucial phenomenon in high-performance devices such as pulse detonation engines and is also relevant in industrial backpressure events that lead to the formation of shock structures within ducts, shock tubes, or nozzles [17–19]. A normal shock wave involves an abrupt conversion of kinetic energy into internal energy, which causes an instantaneous and substantial rise in static pressure and temperature across the discontinuity [20]. This phenomenon induces intensified heat and mass transfer between the superheated gas and the liquid phase (i.e., droplets) downstream of the shock, which causes rapid vaporization of the droplets [5,21–23]. This vaporization often is the crucial first step for reaction initiation in combustion and detonation applications [10,13]. Normal shocks are common in particle-laden flows, including propulsive flows with fuel droplets, explosions in dusty environments, and safety procedures like injecting water droplets for explosion risk reduction. Specifically, normal shocks occur within the self-sustained detonation waves through spray fuel-vapor systems, a key mechanism in rotating and pulse detonation engines [17–19,24–27]. Under these high-compression conditions, droplet heating and vaporization are confined to the region downstream of the shock [28]. Ambient gas entrainment in this post-shock region causes the spray to become sufficiently diluted, allowing the droplets to receive enough energy from the entrained gas for full evaporation [29]. This evaporation process makes the flow colder (due to the latent heat absorbed), a mechanism that can be utilized to prevent reaction, such as in certain fire suppression applications.

The understanding of the evaporation phenomena of sub-micron droplets passing a normal shock is a significant challenge in the study of detonation problems with reactions in droplet-laden flows. The additional complications associated with the presence of two different phases hinder the identification of the main phenomena and prevent the extraction of general conclusions. Despite previous significant efforts, the current level of understanding of many aspects of shock-spray problems is considerably lower than that of purely gaseous systems. A deficiency that limits the modeling strategies and associated predictive capabilities for two-phase flow systems. The goal of this study is to develop a reliable computational model capable of describing the behavior of high-velocity droplet-laden flows passing through a normal shock, which is applicable in scenarios where the droplets are of very small size, of sub-micron order.

The current study is primarily motivated by the demands of emerging clean energy technologies, notably the supersonic separation of ammonia (NH_3) and hydrogen (H_2) [8,30]. Ammonia is considered an energy-dense, cost-effective, safe, and flexible hydrogen carrier [8,31], offering potential solutions to the challenges associated with hydrogen storage and transportation [32]. When used as a hydrogen carrier, ammonia is first produced from hydrogen and nitrogen, then stored and transported in liquid form, and eventually decomposed via a catalyst into a mixture of hydrogen and nitrogen gases. The produced gas mixture often contains traces of undecomposed ammonia due to the limited efficiency of the catalytic decomposition [33]. The mixture, after removing residual NH_3 and trace water [6], is used for various purposes, including indirect NH_3 fuel cells [34], reductive protective gases, and high-purity H_2 production. Following the catalytic decomposition, the residual ammonia is separated via an additional purification process, which can be accomplished through different methods, one of which is supersonic separation. Common supersonic separators usually consist of a convergent–divergent, i.e., Laval, nozzle, swirlers, collectors, and diffusers (See Figure 1) [35]. As the gas expands through the nozzle, its temperature and pressure drop rapidly, causing the residual ammonia to undergo non-equilibrium condensation into sub-micron droplets. Larger droplets ($d > 1 \mu\text{m}$), formed

as the temperature drops through the nozzle, are thrown toward the walls by the flow swirl. These droplets form a liquid film that is subsequently removed by a wall-mounted collector [36,37]. The residual droplets, which have smaller sizes ($d < 0.1 \mu\text{m}$), escape the separation and evaporate through a stagnant normal shock, occurring in the diffuser (see Figure 1) [30,36]. The position of the normal shock depends on various parameters, including the number of nozzle static vanes, inlet and ambient conditions, etc. [36]. It has been shown that although the maximum liquefied mass fraction that can be achieved is about 60%, no more than 20% of the liquid phase will escape from the separation [36,37]. By increasing the ambient pressure, the normal shock advances upstream, resulting in a decrease in the condensation and separation percentage [30]. Hitherto, the physics of this evaporation phenomenon has not been studied completely. Therefore, analyzing the NH_3 spray evaporation through the shock, including the variation in thermodynamic and two-phase flow properties through the shock, is an important objective of this study.

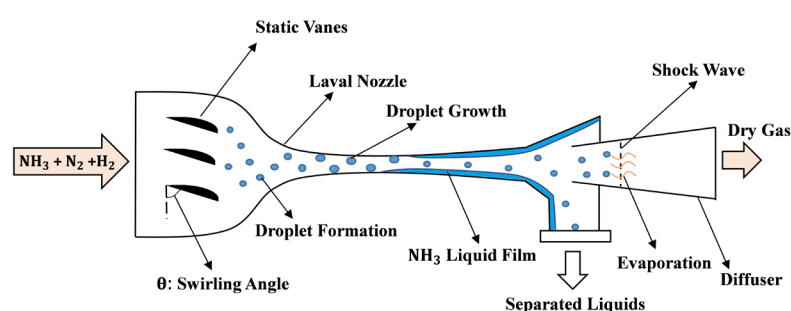


Figure 1. Schematic of supersonic separation of ammonia from $\text{NH}_3 + \text{H}_2 + \text{N}_2$ mixture.

Previous studies have utilized detailed single droplet models [16,38,39] to investigate the droplet parameters and morphology during evaporation in stagnant conditions. However, the use of these detailed methods coupled with the macroscopic conservation equations governing the flow is computationally expensive and time-consuming, making them impractical for large-scale numerical analysis of polydisperse spray evaporation problems. Accordingly, simpler droplet models, such as the Spalding d^2 evaporation law and the Gyarmathy model, are often employed for better computational performance.

The Spalding d^2 evaporation law, coupled with the Clausius–Clapeyron approximation, has been shown to successfully analyze the evaporation in flows containing sprays of fuel droplets during the fuel atomization [1,11,12,14,15]. However, the droplets in these studies are larger than one micron in diameter, and their evaporation regimes are usually under the continuum diffusional regime. The Spalding model assumes that the Lewis number equals one, i.e., that the thermal diffusivity is of the same magnitude as the mass diffusivity, which ensures that the temperature and concentration boundary layers have the same thickness. This leads to a simplified solution for the evaporation rate, based on the assumption that the droplet surface reaches equilibrium conditions quickly relative to the droplet lifetime [40]. However, the Spalding model has been demonstrated not to be sufficiently accurate for post-shock scenarios in nozzle problems, where the droplet diameters are in the sub-micron range [41]. The accuracy of the Spalding model decreases as the droplet size diminishes, because the evaporation regime shifts toward the free-molecular limit (high droplet Knudsen numbers), especially at the final stage of evaporation when the droplets vanish [3,41]. In this free-molecular regime, non-equilibrium effects at the liquid–vapor interface become dominant and the continuum assumption in the Spalding model (implying very low Knudsen numbers) become inconsistent.

Although research in the field of high-speed two-phase flows in the nozzles of supersonic separators [35], steam turbines [42], and thrusters [43] has made great progress, the study of the physics of sub-micron-droplet evaporation during aerodynamic shocks needs

high attention and investigation. The operational, time, and high-cost limitations of experimental methods bolster the role of theoretical studies in analyzing high-speed flows containing droplets. Theoretical approaches in this field include molecular dynamics and computational fluid dynamics (CFD) methods [13,44–47]. CFD methods are divided into two categories: commercial and in-house codes, which are used to analyze the droplet formation and growth problems in flows from a macroscopic perspective and in continuous environments. Commercial codes are usually used to analyze multidimensional problems with turbulent viscosity [20,29,48,49]. These methods have a high computational cost and complexity in the solution convergence. For this reason, one-dimensional in-house codes are recognized as fast and efficient techniques in analyzing the physics governing gas flows containing dispersed droplets. These methods, which usually treat the gas as an inviscid flow, are divided into two categories: semi-analytical (steady) and computational (generally transient) methods [43,46,47]. Semi-analytical methods cannot be extended to multidimensional problems and cannot be equipped with real gas equations in the analysis of aerodynamic shocks. However, computational methods that solve the continuity equations by time-stepping methods do not have those limitations. These methods are suitable options for capturing the aerodynamic shocks and calculating the parameters and energy loss of the flow in the post-shock region. Therefore, this paper presents a novel time-dependent one-dimensional (1D) CFD analysis based on the finite volume method, which is applicable for flows containing sub-micron droplets. This new computational method is used for analyzing the behavior of high-speed droplet-laden flows during and after steady shocks, simultaneously capturing the shock jump and the complex non-equilibrium evaporation processes. Central to the current methodology is the adoption of the Gyarmathy droplet evaporation model [41,50]. This model is capable of simulating droplet evaporation in both diffusion and free-molecular regimes, accurately accounting for the full transition across evaporation regimes. It is thus very suitable for modeling the complete evaporation of diminishing sub-micron droplets. Moreover, a modified version of the Rankine–Hugoniot formulation is derived and used to accurately determine the flow parameters in the fully evaporated condition after the shock.

Due to the similarity in the main physics and as a starting point, the flow considered in this study is assumed to be a single-component NH_3 flow, i.e., a flow where the liquid and vapor phases consist of ammonia only. The diameter of the droplets in the spray is in the sub-micron range, consistent with the droplet sprays at the nozzle outlet of supersonic separators. Therefore, the current modeling utilizes unidirectional coupling for momentum and bidirectional thermodynamic coupling of droplets with the flow. While this approach captures the fundamental impact of latent heat on the gas phase, fully bidirectional coupling (including momentum) would slightly weaken the shock strength while introducing a longer thermal and velocity relaxation zone behind the shock [7]. Furthermore, while the model assumes a monodisperse droplet population, a polydisperse distribution would result in a spatially distributed evaporation process. Because smaller droplets evaporate faster than larger ones, the phase transition region would be lengthened, leading to a more gradual (rather than sharp) recovery of flow parameters downstream of the shock [42]. Finally, although the behavior of real normal shocks deviates from the simplifying assumptions in the 1D model, the latter is a suitable tool for understanding the basic physics behind the studied phenomenon and for quantifying the subsequent complete evaporation process. The insights gained from this analysis will provide a good foundation for the extension of the current 1D CFD study to more complex two-phase droplet-laden flows experiencing a detonation condition with reaction.

2. Problem Definition

A conceptual model of the studied phenomenon is shown in Figure 2. According to this model, a supersonic flow of ammonia vapor, containing a predefined amount of sub-micron droplets of saturated liquid ammonia, experiences a static normal shock, causing a sudden rise in temperature and subsequent rapid evaporation of the droplets. The goal of this study is to analyze the thermodynamic and flow parameters of the sub-micron ammonia spray through and downstream of the shock, and to quantify the evaporation length, i.e., the distance in the post-shock region that is required for complete evaporation. The chosen length of the domain is $x = 45$ mm, whereas the flow is assumed to be one-dimensional, with no change in cross-sectional area. The position of the shock is fixed at $x_{shock} = 20$ mm, and the inlet temperature and pressure are $T_1 = 288.3$ K and $P_1 = 7.3$ bar, corresponding to the saturation state. Hence, the nucleation rate is zero, and the number density of the droplets (i.e., the number of droplets per unit mass) is assumed to be fixed at $n_m = 5 \times 10^{15} \text{ kg}^{-1}$. This assumption does not affect the accuracy of the model even in the fully evaporated region. This is because, under this condition, the droplet radius is very low ($r < r_c$) and the liquid mass fraction is zero. The pre-shock flow is supersonic with a Mach number of $Ma_1 = 1.7$. Four cases for the liquid mass fraction (i.e., the mass of the liquid phase per unit mass of the mixture) are considered: $c_L = 0, 0.02, 0.04$, and 0.08 , designated as cases 1 to 4, respectively.

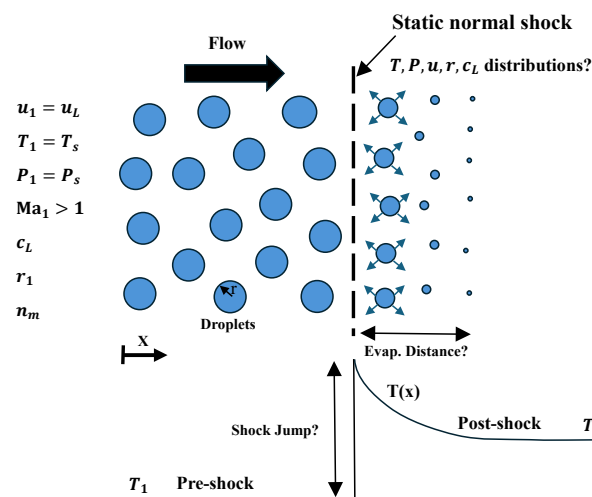


Figure 2. Conceptual model of the evaporation of a sub-micron spray experiencing a normal shock.

2.1. Initial and Boundary Conditions

The initial condition for the pre-shock condition is considered to be the same as the inlet boundary condition, but for the post-shock condition, the suitable initial and boundary conditions are determined using analytical normal shock relations for the two-phase flow, assuming the ideal gas equation of state (see Equations (1)–(3)). These initial values for temperature, pressure, and Mach number for the post-shock conditions are necessary to achieve convergence and keep the shock stable, without moving. The expressions are derived by equating the mass, momentum, and energy expressions before and after the shock jump, assuming full evaporation after the shock. Therefore, the outlet initial value for the post-shock temperature (T_2) is applied by the modified Rankine–Hugoniot formulation for flows containing liquid phase as follows (see Appendix B):

$$\frac{T_2}{T_1} = \frac{1 - \frac{c_L h_{fg}}{C_p T_1} + \frac{\gamma - 1}{2} Ma_1^2}{1 + \frac{\gamma - 1}{2} Ma_2^2} \quad (1)$$

where T_1 is the pre-shock, and T_2 is the post-shock temperature, Ma_1 is the pre-shock, and Ma_2 is the post-shock Mach number. h_{fg} is the latent heat of ammonia at pre-shock conditions, C_p is the isobaric heat capacity of the gas, and γ is the gas isentropic exponent. The outlet pressure and the initial value for the post-shock condition can be derived by equating and solving the equations below to determine Ma_2 and then P_2 numerically (see Appendix B):

$$\frac{P_2}{P_1} = \frac{Ma_1}{(1 - c_L)Ma_2} \sqrt{\frac{1 - \frac{c_L h_{fg}}{C_p T_1} + \frac{\gamma - 1}{2} Ma_1^2}{1 + \frac{\gamma - 1}{2} Ma_2^2}} \quad (2)$$

$$\frac{P_2}{P_1} = \frac{1 + \frac{\gamma}{1 - c_L} Ma_1^2}{1 + \gamma Ma_2^2} \quad (3)$$

The boundary conditions that are applied to the problem for having a fixed normal shock are provided briefly in Table 1. The outlet density and velocity are derived from inner domain cells using first-order Newton extrapolation during the iterations. The outlet temperature is also calculated from the outlet pressure and extrapolated density.

Table 1. Boundary conditions.

Boundary Condition	T	P	u	n	c_L
Inlet	T_1	P_1	u_1	n_m	c_L
Outlet	—	P_2	extrapolation	n_m	0

2.2. Mixture Governing Equations

The conceptual model assumes a one-dimensional, compressible, and inviscid flow. The droplets are assumed to be far apart from each other and homogeneously distributed within the spray, such that the volume fraction of the liquid phase is negligible compared to that of the gas. This indicates a dilute liquid phase with a high void fraction. The governing equations for multi-phase flow consist of conservation laws, equations of state, and models for droplet evaporation. The current Eulerian solvers are computationally efficient for simulating the dominant axial bulk flow variations and the fundamental thermodynamics of spray evaporation. The 1D model governing the conservative equation for a two-phase inviscid flow, based on the Eulerian frame in a fixed cross-section and ignoring diffusional terms, was extended from dry flow principles and follows the time-dependent vector form shown below [41,51].

$$\frac{\partial \vec{Q}}{\partial t} + \frac{\partial \vec{F}}{\partial x} = \vec{S} \quad (4)$$

where x is the horizontal distance from the inlet and t is time. The conservative variables vector $\vec{Q}$ in Equation (4) is defined as follows:

$$\vec{Q} = [\rho \quad \rho u \quad \rho e_t \quad \rho c_L \quad \rho n_m] \quad (5)$$

where ρ is the two-phase flow density, u is the flow velocity, and n_m is the droplet number density. The flux vector ($\vec{F}$) in Equation (4) is defined as follows:

$$\vec{F} = [\rho u \quad \rho u^2 + P \quad \rho e_t u + Pu \quad \rho u c_L \quad \rho u n_m] \quad (6)$$

where P is the flow pressure. The source term vector ($\vec{S}$) in Equation (4) is defined as follows:

$$\vec{S} = \left[\rho u K_A \quad \rho u^2 K_A \quad \rho u h_t K_A \quad 4\pi \rho \rho_L r^2 n_m \frac{dr}{dt} + \rho c_L u K_A \quad \rho n_m u K_A \right] \quad (7)$$

where r is the droplet radius and $K_A = -(dA/dx)/A$ is the flow cross-sectional change coefficient, which in the conceptual model of this study is assumed to be zero ($K_A = 0$). Because of the small Weber number of the droplets ($We_d \ll 12$), the possibility of droplet breaking and coalescence can be ignored [52]. Moreover, since the droplets in this study are assumed to have sub-micron sizes, which yields a small Stokes number ($St_d \ll 1$), a free-slip condition is considered between the phases within the momentum equation [53]. Finally, the total energy e_t in Equation (6) is determined according to the following equation to obtain the flow temperature [54]:

$$e_t = C_v T - c_L h_{fg} + \frac{1}{2} u^2 \quad (8)$$

According to Equation (8), the current model considers the effect of droplet evaporation in the energy conservation equation. Since the temperature and pressure are within a suitable range for assuming ideal gas behavior, the gas properties are described using the ideal gas equation of state and the frozen flow approximation:

$$P = \rho_G R T \quad (9)$$

$$C_p - C_v = R \quad (10)$$

$$\gamma = C_p / C_v \quad (11)$$

Finally, the gas density (ρ_G) is determined from the computed mixture density ($\rho = Q(1)$) as follows [54]:

$$\rho_G = \rho(1 - c_L) / (1 - c_L \rho_L^{-1}) \quad (12)$$

2.3. Liquid Phase Governing Equations

The droplet evaporation rate is determined by calculating the energy transfer between the droplet and the surrounding gas. The traditional evaporation rate for droplets with sizes more than 10 microns is based on the Spalding model as follows [41,55]:

$$\frac{dr}{dt} = - \frac{\lambda_G}{\rho_L C_{p,G} r} \frac{\ln(1 + B_M)}{Le_G} \quad (13)$$

where λ_G is the gas thermal conductivity, B_M is the Spalding mass transfer number, and Le_G is the Lewis number of the gas. In this work, since the droplets are in the sub-micron range, the droplet evaporation rate is determined by the Gyarmathy model, which assumes the temperature inside the droplet to be uniform because of its small size. Employing the Gyarmathy approximation for droplet temperature, the evaporation rate is defined by the Gyarmathy model as follows [41,50,56]:

$$\frac{dr}{dt} = \frac{\alpha_r}{\rho_L h_{fg}} \left(1 - \frac{r_c}{r}\right) (T_s(P) - T) \quad (14)$$

where $T_s(P)$ is the saturation temperature of ammonia at the given pressure. The critical radius of cluster formation r_c is determined as follows [41,57]:

$$r_c = \frac{2\sigma}{\rho_L R T \ln(P/P_s(T))} \quad (15)$$

where $P_s(T)$ is the saturation pressure of ammonia at the given temperature. The convective heat transfer coefficient (α_r), associated with the heat transfer between the droplet and the gas, is given by [41,50,56]:

$$\alpha_r = \frac{\lambda_G}{r \left(1 + \frac{2\sqrt{8\pi}}{1.5\text{Pr}_G} \frac{\gamma}{\gamma+1} \text{Kn}_r \right)} \quad (16)$$

where $\text{Kn}_r = \bar{l}/(2r)$ is the droplet Knudsen number ($\bar{l}$: molecular mean free path distance), and Pr_G is the gas Prandtl number.

The properties of liquid ammonia, including surface tension, droplet density, latent heat, and saturation pressure, are determined as functions of temperature via regression models (see Appendix A), which are based on experimental data found in the literature. The viscosity and the thermal conductivity of gaseous ammonia are functions of temperature and pressure and are determined via the Chung method (see Appendix A) [58].

The computational domain is discretized into control volumes, each of which contains one droplet group, as shown in Figure 3. The equivalent radius of the droplets at the cell center of each control volume is calculated as

$$r = \sqrt[3]{\frac{6c_L}{\pi n_m \rho_L}} \quad (17)$$

where c_L is the liquid mass fraction, ρ_L is the liquid phase density, and n_m is the number density of the droplets.

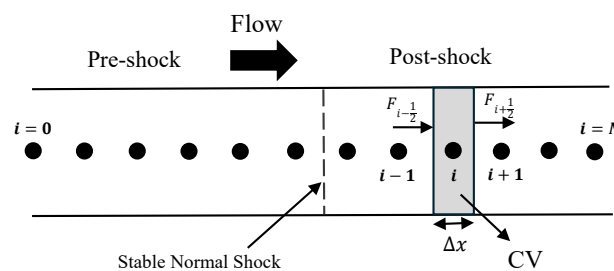


Figure 3. Schematic of the domain discretization.

2.4. Solution Method

The flux terms ($\vec{F}$) are discretized using the Advection Upstream Splitting Method (AUSM), which is well-suited for capturing shocks and steep gradients inherent in gas flows. The temporal discretization is based on an explicit one-step algorithm. The computational domain is divided into $N = 1000$ control volumes, and the conservation equations are solved simultaneously with the droplet evaporation model. The updated conservative vector for the i^{th} - cell center ($\vec{Q}_i^{n+1}$) is determined by calculating the surface flux terms $\vec{F}_{i\pm\frac{1}{2}}^n$ and utilizing the previous time step's conservative vector ($\vec{Q}_i^n$), as follows [59]:

$$\vec{Q}_i^{n+1} = \vec{Q}_i^n - \frac{\Delta t}{\Delta x} \left(\vec{F}_{i+\frac{1}{2}}^n - \vec{F}_{i-\frac{1}{2}}^n \right) + \vec{S}_i^n \Delta t \quad (18)$$

At each time step (n), temperature and pressure are updated from the conservation vector components. The ideal gas equation of state is used to calculate the gas pressure, and subsequent parameters are derived from these updated values. The droplet evaporation source term ($S(4)$) is non-zero during the evaporation.

The iterations continue until the following convergence condition is satisfied:

$$\sum_{i=1}^N \frac{|P_i^{n+1} - P_i^n|}{P_i^n} < \varepsilon \quad (19)$$

where N is the total number of elements. At the n^{th} -time step, the pressure at the center of the i^{th} -element is denoted as P_i^n . The chosen value for the convergence criterion is $\varepsilon = 10^{-6}$. The subsequent time step (Δt) is determined by the following equation:

$$\Delta t = \left(\frac{\Delta x}{u_{max}} \right) \text{CFL} \quad (20)$$

where Δx is the element length and the Courant number (CFL) is assumed to be 0.4. The flowchart of the solution method is presented in Figure 4. The algorithm is implemented in Fortran 90.

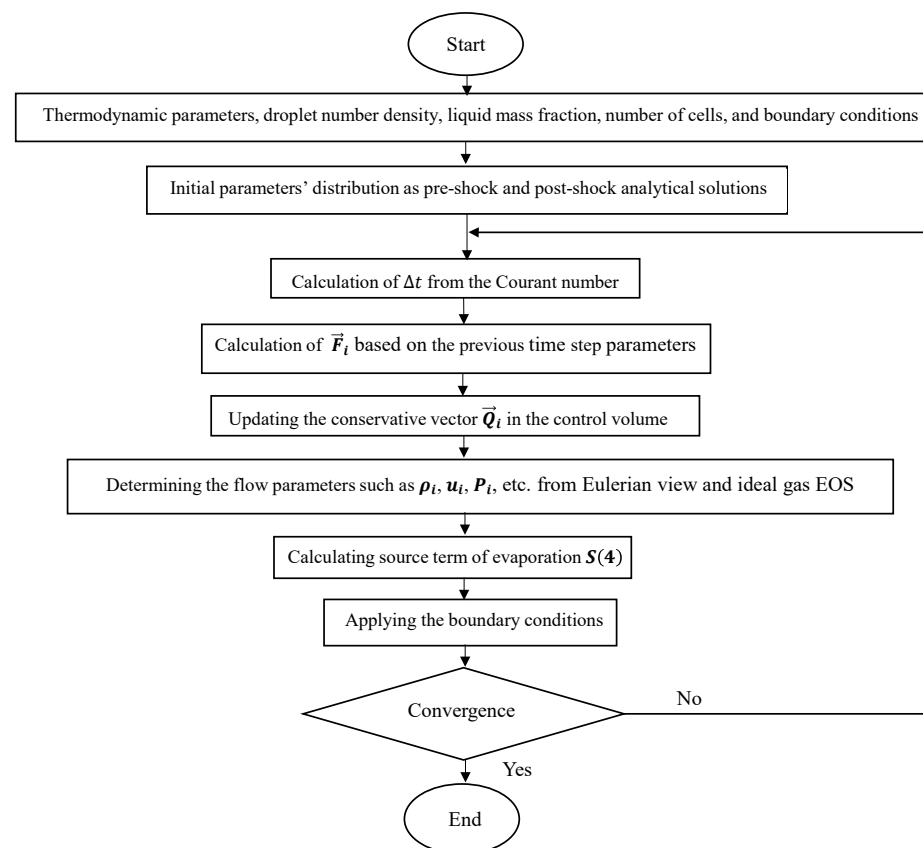


Figure 4. Solution flowchart for the numerical algorithm.

3. Results and Discussion

3.1. Validation Against Experimental Data

Due to the lack of experimental data on normal shocks and droplet evaporation in shock-spray flows involving sub-micron droplets, the validations for two-phase flow pressure, droplet growth, and shock capturing in nozzle flows were performed separately. In the nozzle problems, unlike the shock-spray problems, the variation in channel area is considered. Since the rates of change in droplet size during condensation and evaporation follow identical models, with opposite mathematical signs, validating the growth model during condensation effectively validates the evaporation rate model.

In Figure 5, the 1D model was further applied to the experimental IWSEP nozzle flow ($P_0 = 100$ kPa, $T_0 = 423.6$ K, and $L = 133$ mm) to validate the code in predicting the parameters of a flow experiencing droplet formation in a real problem [60]. The Gyarmathy model presents very good agreement with the experimental data for the pressure distribution along the nozzle's central axis. According to Figure 5, while the trend and the predicted droplet diameters fall within the acceptable experimental range [60], the normalized mean absolute error of 25% indicates a deviation. This order of deviation is accepted

in the literature. In contrast, the Spalding growth model failed to predict the location of condensation shock in the pressure distribution. It has an error of 10.5% in predicting the condensation shock pressure relative to the experimental data of Zhang et al. [60], and the resulting sub-micron droplet sizes are not in the acceptable experimental range, with a normalized mean absolute error of 65%. The errors of Gyarmathy's model are likely attributable to the limitations of the current single-diameter 1D model, which neglects the droplet size-distribution. Other contributing factors may include the inviscid flow assumption, disregard of inter-phase slip flow and droplet coalescence, neglecting the two-way momentum coupling between the phases, stagnant flow assumption governing the nucleation model, and inherent limitations in the accuracy of the experimental droplet size measurements.

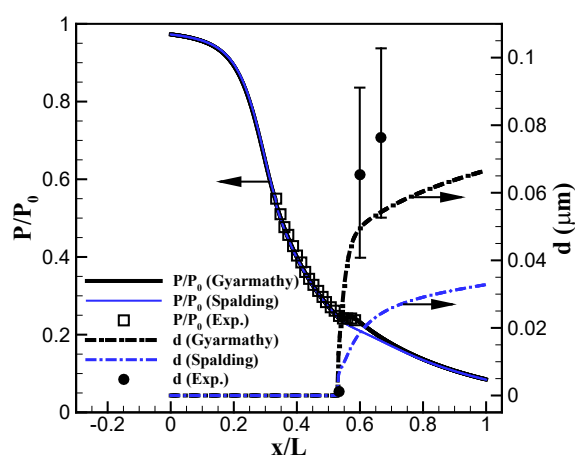


Figure 5. Validation of the pressure and droplet diameter variation with Zhang et al. experimental data [60] ($P_0 = 100$ kPa, $T_0 = 423.6$ K, and $L = 133$ mm).

To have a comparing view between the results considering Gyarmathy, and Spalding growth model with numerical solution of ANSYS Fluent 19.1, the contour of the pressure and droplet radius through the Moore Nozzle B along with the average of their value in each nozzle section in the divergent part are presented in Figure 6. As it is obvious, employing the Gyarmathy model provides a more similar trend with the ANSYS Fluent solution data of pressure and droplet diameter than the Spalding model. Moreover, although the normalized mean absolute error for determining the pressure distribution using Gyarmathy and Spalding growth models are 6.1% and 4.05%, the errors in determining the droplet radius are 39.5% and 85.6%, respectively. This shows that the Gyarmathy model generally offers better accuracy and more realistic behavior when predicting the parameters of two-phase flows containing sub-micron droplets. The reason for this difference is that ANSYS Fluent 19.1 solves the problem two-dimensionally, employs the virial equation of state, and employs Hill's growth model throughout the solution [61]. Moreover, the pressure and droplet radius data from ANSYS Fluent have been determined by averaging at each section to obtain distortion-free data in the x-direction through the nozzle. This makes some deviations between the solution data from ANSYS Fluent and the data from 1D models.

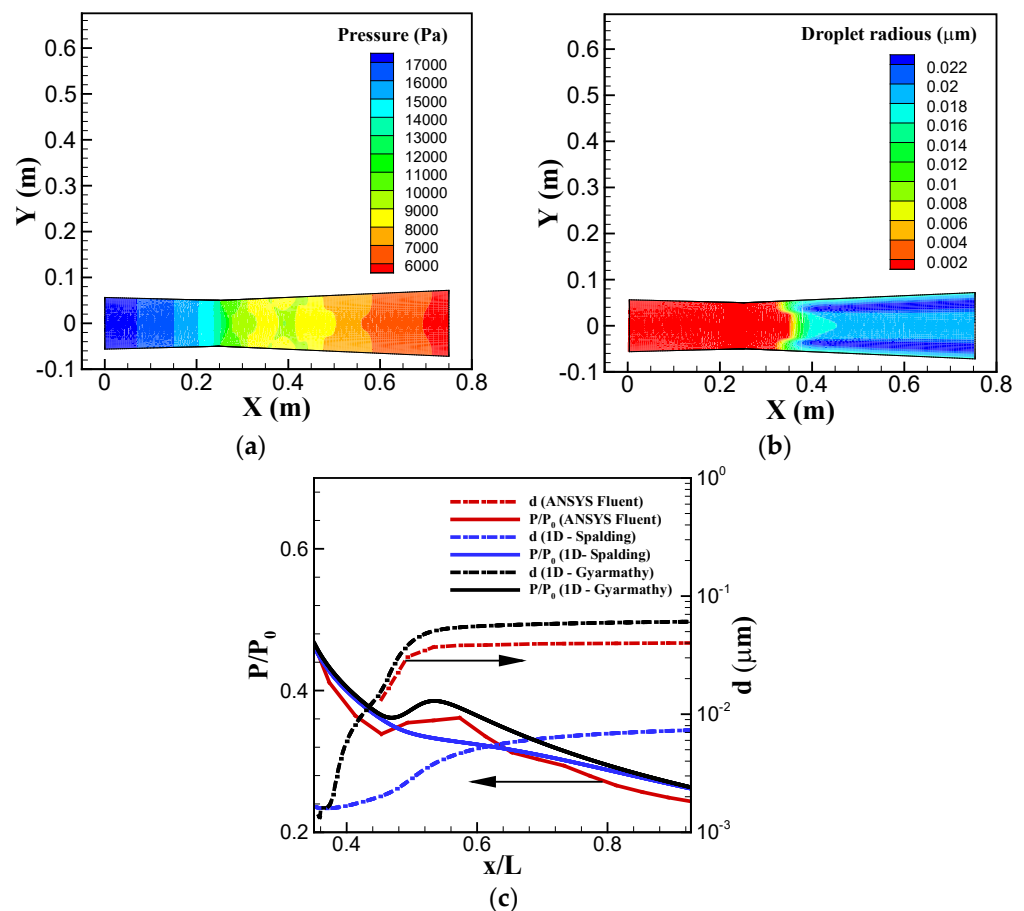


Figure 6. Contours of (a) pressure and (b) droplet radius through the Moore nozzle using ANSYS Fluent. Comparing the pressure and droplet sizes resulting from the current model with numerical solution of ANSYS Fluent at each section of (c) Moore et al. nozzle [62] for water steam ($P_0 = 25$ kPa, $T_0 = 357.6$ K, $L = 750$ mm).

To verify the accuracy of the model in shock capturing, the distribution of the air flow density calculated by the current model has been compared with the numerical solution data of Arina when $P_0 = 10^5$ Pa, $T_0 = 288$ K, and $P_{ex} = 8.3 \times 10^4$ Pa [63] in Figure 7. The normalized mean absolute error of the current model against Arina's numerical solution is 3.1%, which shows a good agreement. Moreover, to verify the model's accuracy in predicting two-phase parameters during evaporation through shocks, the flow temperature at fully evaporated outlet conditions is compared with the modified two-phase Rankine-Huguenot analytical solutions in Figure 8a. As shown, there is a strong agreement between the model results and the analytical solutions. This also confirms the model accuracy in predicting evaporation during the shocks.

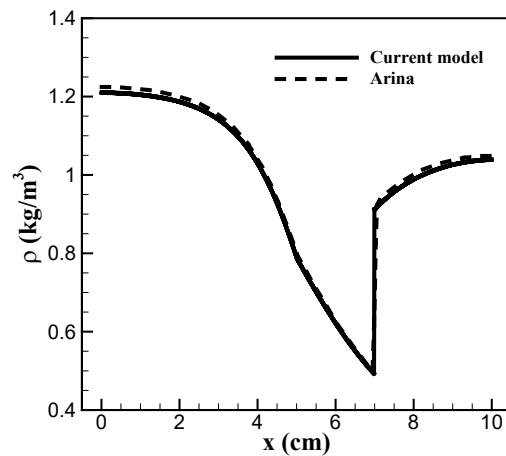


Figure 7. Verification of the flow density calculated by the current numerical model against Arina's solution [63] for air experiencing a normal shock ($P_0 = 10^5$ kPa, $T_0 = 288$ K, and $P_{ex} = 8.3 \times 10^4$ Pa).

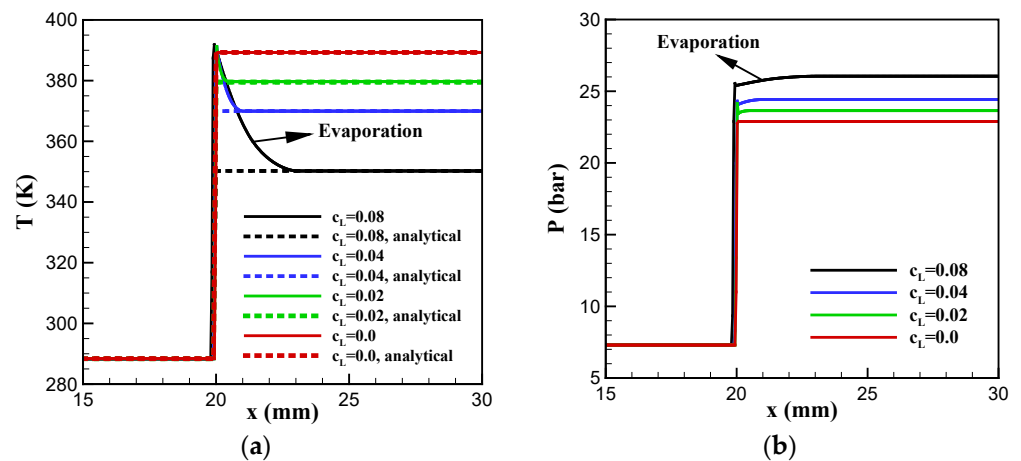


Figure 8. Distribution of flow (a) temperature and (b) pressure through the normal shock.

3.2. Phase Diagram Analysis

According to Figure 9, for all cases, the inlet condition was selected to be on a saturation state, the equilibrium condition, which is usually provided at the final sections of the supersonic separator nozzle [41]. This makes the inlet under the condition without evaporation or condensation. During the shock, the state condition jumped to the superheat region where the droplets start evaporation rapidly and absorb energy from the flow, making the flow cooler and increasing the pressure due to the Rayleigh effect. By increasing the mass fraction of the droplets in the flow, the reduction in temperature and enhancement in the pressure due to the evaporation will be stronger.

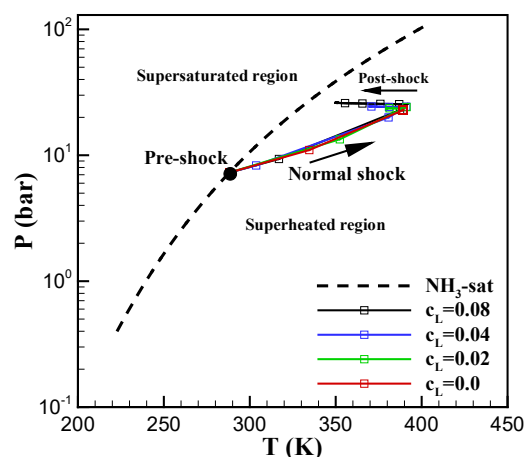


Figure 9. Phase diagram for the evaporation process during the normal shock.

3.3. Analysis of the Evaporation Process

In Figure 10a–c, the droplet radius, evaporation rate, and liquid mass fraction variation are shown in the pre-shock and after the shock region. The number density of the droplets remained fixed during the shock. This is because the flow state does not enter supersaturation conditions, and the nucleation rate is zero during the evaporation process. The Knudsen number of droplets will increase from $Kn_r = 0.03$ (diffusion regime) to a maximum of $Kn_d = 27$ (transition and free-molecular regimes) across the shock, reinforcing the importance of the Gyrnathy modification and the transient regime across the shock. According to Figure 10a, the evaporation has four stages. At first, the negative evaporation rate increases abruptly (stage 1), then it remains fixed during a short period (stage 2), and increases in a stronger reduction (stage 3), finally it decreases abruptly to finish the evaporation process, and the droplet spray completely disappears (stage 4). As is obvious, by increasing the liquid content in the flow from $c_L = 0.02$ to $c_L = 0.08$, the evaporation period is lengthened from 0.5 mm to about 3 mm (see Figure 10a,c). However, the abrupt enhancement in evaporation rate during stage (3) decreases from $dr/dt = -28$ cm/s to $dr/dt = -10$ cm/s. Figure 10b shows the variation in droplet size through the normal shock. According to the figure, the droplets' size first experiences a local expansion for a short period because of an abrupt reduction in the density of liquid droplets through the shock (see Equation (14)), then it will decrease to zero afterwards due to evaporation. This means that, in the initial stages of shock, the effect of droplet expansion due to density reduction is greater than the effects of heat and mass transfer during evaporation. Therefore, the droplets' radius increases locally. This increase in size, also called initial droplet inflation, has been observed in many time-dependent analyses and experimental investigations of single and stagnant droplet evaporation [16,21,38]. According to Figure 10, the maximum droplet swelling due to shock is 17%, corresponding to larger droplet sizes at the inlet. Increasing the liquid mass fraction (droplet size) in the flow enhances local swelling. This is because the evaporation rate is lower in flows with higher liquid content due to the inverse relationship between evaporation rate and droplet radius (see Equations (14) and (16)). Therefore, the droplets swell more during the initial stages of normal shock.

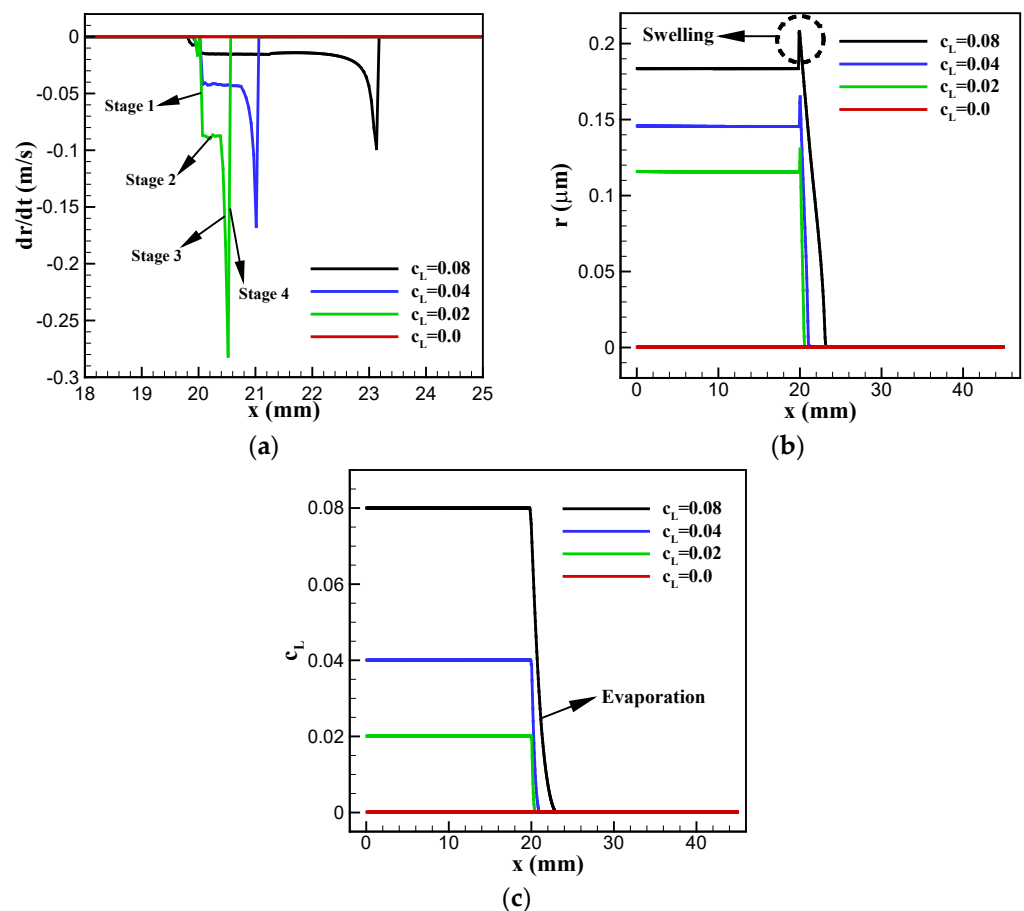


Figure 10. Variation of (a) evaporation rate, (b) droplet radius, and (c) liquid mass fraction through the shock.

3.4. Analysis of the Flow Thermodynamics

The distribution of temperature and pressure of the flow is shown through the pre- and post-shock regions in Figure 8a,b. As can be seen, the jump in the temperature for all numerical solution cases is approximately the same, even with no content of the liquid phase. However, the pressure jump of the flow during the shock is higher for the cases with a higher content of the liquid phase. For instance, the pressure jump of the case containing 8% liquid phase is approximately 13% more relative to the case without liquid content. As illustrated, the numerical solution predicts a higher temperature jump than the analytical solution. Accurately determining the jump temperature is useful for verifying the potential for detonation. Additionally, correctly determining the jump leads to an accurate determination of droplet swelling, which cannot be achieved through an analytical solution. In other words, the analytical solution yields a zero size or complete evaporation after the shock, as well as infinite evaporation at the jump point, neither of which is correct.

Due to the evaporation, the flow temperature decreases significantly (about 50 K for the case with 8% liquid phase) with longer evaporation distance. As it is obvious, the evaporation distance is at max 3 mm for the case with 8% droplets. It is obvious from Figure 8a that the analytical solution cannot predict the jumping in the two-phase temperature and evaporation region well. However, the computational solution and analytical solutions will overlap in the region far from the shock where the droplets are fully evaporated. This is because the gas has been assumed to have frozen properties with the ideal gas EOS in both numerical and analytical solutions. This results in a unique solution for numerical and analytical solutions in the fully evaporation region. Otherwise, the

shock will move along the domain during the solution, and the convergence will not be achieved. The reduction in temperature due to evaporation during the post-shock can prevent the potential for reaction in the more complex flows containing fuel droplet-oxidant flows. This is because, during the evaporation, the droplet absorbs heat and decreases the temperature of the flow. During this process, the pressure will increase because of the Rayleigh effect during heat release in the subsonic flow. When the droplet spray is completely evaporated and disappears, the pressure and the temperature experience no change in the post-shock region.

3.5. Analysis of the Flow Dynamics

Evaporation affects the flow dynamics. The normal shock makes the flow slower and compressed. Figure 11a,b show the Mach number and velocity distribution of the two-phase flow for various cases through and after the normal shock. As can be seen, the jump in the Mach number and velocity through the shock is stronger for the cases with a higher content of the liquid phase. Moreover, due to the evaporation, the flow speed will decrease due to the heat absorption, which applies the Rayleigh effect to the flow. Therefore, the cases with higher liquid phase contents have a lower Mach number and velocity at the outlet. It is worth mentioning that the sensitivity of the velocity reduction to the liquid phase content is more than the Mach number.

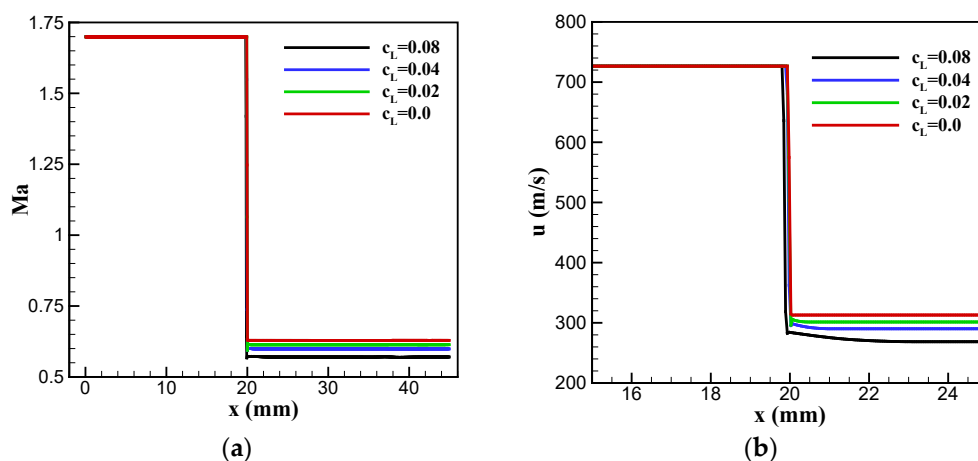


Figure 11. Distribution of flow (a) Mach number and (b) velocity through the normal shock.

4. Concluding Remarks

This study successfully employed a novel time-dependent one-dimensional CFD model to analyze the complex, non-equilibrium evaporation of a sub-micron droplet spray subjected to a stationary normal shock. By incorporating the comprehensive Gyarmathy model and a modified two-phase jump formulation for the normal shock, the model accurately addresses the limitations of conventional approaches, such as the Spalding d^2 -law, for the free-molecular regime and sub-micron droplet spray evaporation. The analysis confirmed that the normal shock is a critical transition mechanism, instantaneously jumping the flow from a supersaturation state to a superheated state, which drives droplet evaporation. The evaporation process through normal shocks proceeds through four distinct stages, culminating in the complete evaporation of the droplet over a short distance (max 3 mm). Crucially, the droplets experience a 17% local short-period swelling in size through the shock, which decreases by liquid content in the flow. Moreover, the initial liquid mass fraction greatly influences the post-shock flow dynamics. It will lengthen the evaporation region and decrease the maximum evaporation rate. It has also been shown that increased droplet content significantly enhances the thermodynamic

response. For example, an 8% liquid mass fraction increased the pressure jump across the shock by approximately 13% compared to the dry flow. This resulting heat absorption induces the Rayleigh effect, causing substantial vapor cooling (up to 50 K) and a significant decrease in flow velocity and Mach number downstream. In conclusion, the current CFD model provides high-fidelity, quantitative insights into the fundamental physics governing sub-micron droplet behavior during shock compression. The findings are vital for optimizing emerging technologies, such as NH_3 supersonic liquefaction, and establishing a robust foundation for modeling complex, multidimensional two-phase detonation flows.

Author Contributions: Investigation, M.S.; Resources, M.S., A.T.; Software, M.S.; Writing—Original Draft, M.S.; Methodology, M.S., H.G.; Conceptualization, H.G., A.T., K.F., G.P.; Validation, M.S., H.G., K.F.; Data curation, M.S.; Writing—Review and Editing, H.G., A.T., K.F., G.P., B.S., M.I.; Formal analysis, H.G., A.T., K.F., G.P., B.S., M.I.; Supervision, H.G., A.T. All authors have read and agreed to the published version of the manuscript.

Funding: This study is financed by the European Union—NextGenerationEU—through the National Recovery and Resilience Plan of the Republic of Bulgaria, Project No. BG-RRP-2.004-0005.

Data Availability Statement: Data will be made available on request.

Acknowledgments: M. Sahami would like to express his deep gratitude to the Technical University of Sofia for the opportunity to carry out a postdoctoral research fellowship. M. Sahami also wants to acknowledge Universidad Politécnica de Madrid for supporting him during an Erasmus+ research visit under Project No. 2020-1-ES01-KA107-080401 in 2022 to produce a part of the results in this study.

Conflicts of Interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Nomenclature

A	Channel cross-sectional area, m^2
B_M	Spalding mass transfer number
c_L	Liquid mass fraction
C_p	Gas isobaric specific heat capacity, $\text{J}/(\text{kg} \cdot \text{K})$
C_v	Gas isochoric specific heat capacity, $\text{J}/(\text{kg} \cdot \text{K})$
d	Diameter of droplets, μm
e	Specific internal energy of two-phase flow, J/kg
$\vec{F}$	Vector of surface flux
h	Specific enthalpy of two-phase flow, J/kg
h_{fg}	Latent heat of evaporation per unit mass, J/kg
Kn	Knudsen number
K_A	Cross-sectional change coefficient, $1/\text{m}$
L	Channel length, m
$\bar{l}$	Length of free molecular mean path, m
Le_G	Lewis number of gas
m	Mass, kg
$\dot{m}$	Mass flow rate, kg/s
M	Molar mass, kg/mole
Ma	Mach number
N	Total number of control volumes
n_m	Total droplets number density, $1/\text{kg}$
P	Static pressure, Pa
Pr_G	Prandtl number of the gas
P_s	Saturation pressure, Pa
P_v	Vapor pressure, Pa
$\vec{Q}$	Conservative variable vector

$Q(1)$	First component of conservative vector
R	Gas constant, J/(kg.K)
r	Droplet radius, μm
$\vec{S}$	Source term vector
S_p	Supersaturation degree
St	Stokes number
T	Flow temperature, K
t	Time, s
u	Flow velocity, m/s
V	Volume, m^3
v	Specific volume, m^3/kg
We	Weber number
x	Axial distance from domain inlet, m
Greek letters	
α_r	Heat transfer coefficient, $\text{W}/(\text{m}^2 \cdot \text{K})$
Δt	Time step, s
Δx	Length of control volume, m
ε	Convergence criterion
γ	Isentropic exponent of gas
λ_G	Thermal conductivity, $\text{W}/(\text{m} \cdot \text{K})$
μ	Dynamic viscosity, Pa.s
ρ	Density of two-phase mixture, kg/m^3
σ	Surface tension, N/m
Subscripts	
1	One vapor molecule, pre-shock state
2	Post-shock state
c	Critical
d	Droplet
G	Gaseous phase
L	Liquid phase
i	Elements index
max	Maximum
N	Total number of elements
n	Time step index
nuc	Nucleation
r	Droplet radius
s	Saturation
t	total
v	Vapor
0	Channel inlet stagnation condition, Ideal gas
Abbreviations	
<i>AUSM</i>	Advection Upstream Splitting Method
<i>CFL</i>	Courant-Friedrichs-Lewy number
<i>CFD</i>	Computational Fluid Dynamics
<i>CV</i>	Control Volume
<i>EOS</i>	Equation Of State
<i>IWESP</i>	International Wet Steam Experimental Project
<i>1D</i>	One Dimensional

Appendix A. Physical Relations for the Liquid and Gaseous Phases

Using existing data [54], a polynomial relationship between ammonia saturation pressure P_s and temperature T is determined as follows:

$$P_s = a_0 + a_1T + a_2T^2 + a_3T^3 + a_4T^4 \quad (\text{A1})$$

where T and P_s are in Celsius and bar, respectively. The coefficients a_0 to a_5 for various temperature ranges are presented in Table A1.

Table A1. Coefficients for calculation of the saturation pressure in Equation (A1).

	a_0	a_1	a_2	a_3
$-50\text{ }^\circ\text{C} \leq T < -6\text{ }^\circ\text{C}$	4.240234	0.1520876	0.0019527	0.000008893
$-6\text{ }^\circ\text{C} \leq T < 64\text{ }^\circ\text{C}$	4.297223	0.1615944	0.0022271	0.000019118
$64\text{ }^\circ\text{C} \leq T < 132\text{ }^\circ\text{C}$	-5.39522765	0.5250517	-0.002388	0.0000392712

The density of liquid NH_3 (in kg/m^3) is assumed to be a function of temperature, and it is correlated by Equation (A2) [54]:

$$\rho_L = a_0 + a_1T + a_2T^2 + a_3T^3 \quad (\text{A2})$$

where T is in Kelvin. The coefficients a_0 to a_3 are presented in Table A2.

Table A2. Coefficients for calculating the density of liquid NH_3 by Equation (A2).

a_0	a_1	a_2	a_3
638.9391809947	1.337287169	-0.0026840395	-0.0000195513

To calculate the surface tension of NH_3 droplets (in N/m), Equation (A3) is used [64]:

$$\sigma = a_0 \left(1 - \frac{T}{T_c}\right)^{a_1} + a_2 \left(1 - \frac{T}{T_c}\right)^{a_3} \quad (\text{A3})$$

where T is in Kelvin and T_c is the critical temperature of ammonia. The coefficients a_0 to a_3 are presented in Table A3.

Table A3. Coefficients for calculating the surface tension of liquid NH_3 by Equation (A3).

a_0	a_1	a_2	a_3
0.1028	1.211	-0.09453	5.585

The latent heat of ammonia has been assumed to be fixed ($h_{fg} = 1200\text{ kJ/kg}$) corresponding to the pre-shock temperature for the provision of the stable shock during the computational solution.

In the AUSM scheme, the flow Mach number for flux calculations is determined by

$$\text{Ma} = \frac{u}{\sqrt{\gamma P / \rho_G}} \quad (\text{A4})$$

where γ is the isentropic exponent of the gas and u is the flow velocity. The Chung method [58] is employed to accurately calculate the dynamic viscosity μ_G and thermal conductivity λ_G of the gas.

$$\mu_G(T, \rho_G) = \mu_g^* \frac{36.344 \sqrt{m_1 T_c}}{v_c^{2/3}} \quad (\text{A5})$$

$$\lambda_G(T, \rho_G) = \frac{31.2 \mu_0 \psi}{M} (G_2^{-1} + B_6 \tilde{y}) + q B_7 \tilde{y}^2 \sqrt{T_r} G_2 \quad (\text{A6})$$

Equations (A5) and (A6) include the gas equivalent molecular mass (m_1), critical temperature (T_c), and reduced temperature (T_r) with all other parameters (such as μ_0 , ψ , G_2 , $\tilde{y}$, v_c , etc.) derived as per a previously recommended methodology [58].

Appendix B. Derivation of Modified Rankine–Hugoniot Expressions

Appendix B.1. Energy Conservation Analysis

The total energy of the flow $h_{t,1}$ before the shock is defined as follows:

$$\dot{m}h_{t,1} = \dot{m}_{G1} \left(h_{G1} + \frac{u_{G1}^2}{2} \right) + \dot{m}_L \left(h_L + \frac{u_L^2}{2} \right) \quad (\text{A7})$$

where $\dot{m}$ is the total mass flow rate, $\dot{m}_{G1}$ is the gas phase mass flow rate, h_{G1} is the enthalpy of the gas phase, $\dot{m}_L$ is the mass flow rate of the liquid phase, h_L is the enthalpy of the liquid phase and u_L is the velocity of droplets in the pre-shock conditions. Assuming $u_{G1} = u_L = u_1$, $\dot{m}_G/\dot{m} = (1 - c_L)$, $\dot{m}_L/\dot{m} = c_L$, $h_{G1} - h_L \approx h_{fg}$, and $h_G = C_p T$, the following expression can be written for the total enthalpy in the pre-shock conditions [65,66]:

$$h_{t,1} = C_p T_1 - c_L h_{fg} + \frac{u_1^2}{2} \quad (\text{A8})$$

where C_p is the isobaric heat capacity of the gas, c_L is the liquid phase mass fraction, u_1 is the flow velocity, h_{fg} is the latent heat of evaporation, and T_1 is the flow temperature in the pre-shock region (index 1 shows the flow state at pre-shock conditions). Similarly, for the post-shock condition where the flow is dry, the total enthalpy can be driven as follows:

$$h_{t,2} = C_p T_2 + \frac{u_2^2}{2} \quad (\text{A9})$$

where index 2 shows the flow state in the post-shock conditions. Since normal shock is adiabatic, according to the first law of thermodynamics, the total enthalpy will remain fixed through the normal shock ($h_{t,1} = h_{t,2}$). Therefore, by equating Equations (A8) and (A9) and using the Mach number definition $\text{Ma} = u/\sqrt{\gamma RT}$, the modified Rankine–Hugoniot expression for post-shock temperature of a two-phase flow will be derived as follows:

$$\frac{T_2}{T_1} = \frac{1 - \frac{c_L h_{fg}}{C_p T_1} + \frac{\gamma - 1}{2} \text{Ma}_1^2}{1 + \frac{\gamma - 1}{2} \text{Ma}_2^2} \quad (\text{A10})$$

Appendix B.2. Mass Conservation Analysis

Assuming full evaporation after shock, the mass conservation through the shock can be written as follows:

$$\dot{m}_{G1} + \dot{m}_L = \dot{m}_{G2} \quad (\text{A11})$$

where $\dot{m}_L$ is the mass flow rate of the flow in the pre-shock conditions. Applying $\dot{m}_{G1} = (1 - c_L)\dot{m}$ and $\dot{m}_L = c_L\dot{m}$, the following expression for mass flow rate after the shock $\dot{m}_{G2}$ will be derived as a function of gas part mass flow rate before the shock:

$$\dot{m}_{G2} = \frac{\dot{m}_{G1}}{(1 - c_L)} \quad (\text{A12})$$

where $\dot{m}_{G1} = \rho_1 u_1 A$ (A is the flow cross-section area). Rewriting Equation (A11) based on inlet gas state, using the ideal gas EOS for the inlet gas density $\rho_1 = P_1/(RT)$, applying Mach number definition $\text{Ma} = u/\sqrt{\gamma RT}$, then substituting Equation (A10), the following modified Rankine–Hugoniot expression for the pressure after the normal shock will be achieved:

$$\frac{P_2}{P_1} = \frac{Ma_1}{(1 - c_L)Ma_2} \sqrt{\frac{1 - \frac{c_L h_{fg}}{c_p T_1} + \frac{\gamma - 1}{2} Ma_1^2}{1 + \frac{\gamma - 1}{2} Ma_2^2}} \quad (A13)$$

Appendix B.3. Momentum Conservation Analysis

Using the conservation of momentum through the normal shock, the following expression will be derived:

$$P_1 - P_2 = \frac{\dot{m}_{G2}u_2 - \dot{m}u_1}{A} \quad (A14)$$

By applying $\dot{m}_{L1} = c_L \dot{m}$ and $\dot{m} = \dot{m}_{G1}/(1 - c_L)$, then $\dot{m}_{G1} = \rho_1 u_1 A$, Equation (A14) can be rewritten as follows:

$$P_1 + \frac{\rho_1 u_1^2}{1 - c_L} = P_2 + \rho_2 u_2^2 \quad (A15)$$

By considering $Ma = u/\sqrt{\gamma RT}$, considering ideal gas EOS, $\rho_1 = P_1/(RT)$, and some rearranging, Equation (A15) will be written as follows as another analytical expression for outlet pressure:

$$\frac{P_2}{P_1} = \frac{1 + \frac{\gamma}{1 - c_L} Ma_1^2}{1 + \gamma Ma_2^2} \quad (A16)$$

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