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# An Investigation of the Growth of Particles Produced in a Laval Nozzle

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*This study is focused on numerical modeling of condensation of water vapor in a Laval nozzle, using the liquid drop nucleation theory. Influence of nozzle geometry, pressure and temperature on the average drop size is reported. A computer program written in MATLAB has been used to calculate the nucleation and condensation of water vapor in the nozzle. The simulation results are validated with the available experimental data in the literature for steam condensation. The model reveals that the average drop size is reduced by increasing the divergent angle of the nozzle. The results also confirm that increasing the inlet pressure has a direct effect on the average drop size while temperature rise has an inverse effect on the drop size.*

**Keywords:** Laval nozzle, MATLAB, Nucleation and condensation, Numerical modeling.

## 1. Introduction

The convergent-divergent (Laval) nozzle had the most pervasive application in military issues as well as the missile and rocket launching in the last century. However, in the early decade it has found application in production of nano-particles such as magnesium and composite vapour deposition (CVD) diamond. One of the major applications for Laval nozzles is production of fine metallic particles. Supersonic quenching of metallurgical gases used to produce fine metallic particles in large quantities. This process starts by rapid condensation of a supersaturated metallic vapor in Laval nozzle (Brooks *et al.*, 2006). In the nozzle, shock wave with a sharp drop in temperature causes the growth of nuclei. The particle size of the nano-materials using the nucleation and condensation generation phenomena will grow along the nozzle to reach the desired size. At the end of the nozzle particles should be reached to the desired size. Various factors have an effect on particle size such as nozzle divergent angle, inlet pressure and temperature (Brooks *et al.*, 2006). The current research of Brooks *et al.* (2006) describes the production of magnesium using a laval nozzle. There is

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reported research work for use of shock waves to increase the size of Chemical Vapor Deposition (CVD) diamond nuclei as well (Sung & Lin, 2010). Condensation phenomena causes that new critical nuclei grow along the nozzle to reach the desired size. Describing this phenomenon is expressed as simply the process of converting gas changing to liquid. The initiation of the condensation process is conventionally related to nucleation (Sidin, 2009). Condensation not only takes place in atmospheric clouds but also in turbine and nozzle (Binnie & Green, 1942; Hill *et al.*, 1963; Kremmer & Okurounmu, 1965; Moses & Stein, 1978). In addition, there are treatments on the general condensation process including studies on the thermodynamics of droplet nucleation and growth. The mathematical model is essential for design of the nozzle and also to find the suitable operating conditions for the production of particles in the desired size range. One of the examples is condensation of water vapour in the Laval nozzle. However, water physical and thermodynamics properties are easy to find and also there are experimental results on water condensation such as Binnie and Green, (1942) and Hill *et al.* (1963 and 1966). Current research, water particles size was modeled based on fundamental equations of fluid motion, air ideal gas equations and nucleation and condensation equations in one dimensional system based on length of the nozzle. Finally, model is validated by experimental results available in the literature. The prediction of particle size by model has good agreement with the experimental data. For the next step, model can be extended to cover other components such as CVD diamond, MgO and non-metallic vapours.

However, there is no reported work in literature on the effects of operating conditions such as pressure and temperature on the growth of droplets.

This study is focused on the fundamental dynamics and thermodynamics of the simultaneous condensation and expansion process. The specific objective of this work is to examine the differences between theoretical and experimental expansion of initially saturated water vapors. The following parameters have been considered in this modeling. Firstly, the effect of the nozzle divergent angle is studied to optimize the drop radius. Then, the effects of inlet pressure and temperature on condensation and average drop radius in the nozzle have been investigated.

## **2. Literature review**

Theoretical prediction for the condensation phenomenon was initially started in 1942 (Oswatitsch, 1942). They have yielded encouraging agreement between experimental data and existing nucleation theory that it seemed legitimate to apply a similar procedure to the expansion of metal vapors in the turbine nozzles (Hill *et al.*, 1963).

Equations describing the nucleation phenomenon were derived using the classical approach for each species in the system, at the flow temperature and its partial pressure. The partial pressure was found using Dalton's law. The equations which describe droplet growth (taking place after nucleation has created a droplet of sufficient size) were derived by allowing molecules of any specie which has crossed its vapor pressure curve to stick to the droplets presents in the system. Mass accumulation was accounted for through a mass growth equation (Hill *et al.*, 1963).

Therefore, studies on steam condensation have been conducted as one of the quenching approaches (Binnie & Green, 1942). Laval nozzles have been used to cool gas rapidly at more than  $10^6$  °C/s (Brooks *et al.*, 2006; Hasan *et al.*, 2006). As a result, homogeneous nucleation and condensation of the vapor is facilitated (Kuan & Witt, 2013).

In the field of metallic vapours, a number of researchers (Bayazitoglu *et al.*, 1996; Hill *et al.*, (1963) and Koo *et al.*, 2008), have modelled nucleation and condensation in one-dimensional inviscid compressible flow based on Classical Nucleation Theory (CNT). The major challenge in the supersonic quenching is the size of droplets. In the work of Hill *et al.* (1963), droplets size is in sub-micron range. They investigated nucleation and condensation of metals vapor such as Na, K and Rb (Hill *et al.*, 1963). In the case of Koo *et al.* (2008), droplets size is in the nano-scale range. They have investigated experimentally and numerically nucleation and condensation of Mg vapor that produced in carbothermic reaction of MgO and C. Effect of Mg vapor concentration and inlet temperature and pressure on droplet size have also been modelled (Koo *et al.*, 2008). The work of Bayazitoglu *et al.* (1996), showed nucleation of Zn vapor mixture both experimentally and analytically in a converging nozzle. Influence of different operating conditions and also three different converging angle on weighted average radius have been investigated. In this case the droplet size was in the range of 20 to  $81\mu\text{m}$  (Bayazitoglu *et al.*, 1996).

There are significant experimental works on supersonic quenching of saturated steam in a Laval nozzle. A number of investigations (Binnie & Green, 1942; Heath *et al.*, 2002; Hill,

1966; Wegener & Pouring, 1964; Wyslouzil *et al.*, 2000) have studied conditions give rise to onset of nucleation. A wide range of experiment between -40 to 40°C has been done on onset of condensation in supersonic Laval nozzle by Moses and Stein. in their work, the location of onset point, local rate of nucleation and droplet size measured using laser light scattering technique (Moses & Stein, 1978).

Khan *et al.* (2003) implemented the new method of Small Angle Neutron Scattering (SANS) to characterize nano droplet density and measurement of the nucleation rate of D<sub>2</sub>O in a supersonic nozzle (Khan *et al.*, 2003).

An investigation has been carried out using different models as presented in the work of Sinha *et al.* (2009). They developed a steady state one-dimensional model to examine the formation and growth of H<sub>2</sub>O/D<sub>2</sub>O droplet in a supersonic nozzle. Hale's scaled model used to predict particle formation rate. Five growth laws of isothermal and nonisothermal have been presented and compared with experimental data (Sinha *et al.*, 2009).

Two numerical investigations have been carried out in nucleation and condensation of steam by Yang and Shen (2009) and Yang *et al.* (2010). In the first case, effect of release latent heat during homogeneous nucleation of steam on transonic or supersonic with shock waves flow has been studied. The Virial equation of state was used instead of ideal gas. Consequently, dry isentropic expansion and non-equilibrium were compared (Yang & Shen, 2009). In the second case, influences of condensation shock and normal aerodynamic shock on nucleation and condensation have been investigated (Yang *et al.*, 2010).

Recently, a remarkable researches on quenching of the Mg vapour in the carbothermal reduction process in the Laval nozzle have reported (Kuan & Witt, 2013). Effects of heat transfer, gas turbulence, vapour concentration and type of carrier gas on the particles size has been investigated in the modelling and validated using their own experimental data. Furthermore, gas turbulence and the effect of compressibility were modelled by solving the Reynolds-Averaged Navier-Stokes (RANS) equations (Kuan & Witt, 2013). Effect of different mesh grid and turbulence models in Laval nozzle on heat transfer coefficient have been investigated in recent work of Zhalehrajabi *et al.* (2013).

The major difference between the present work and those reported in literature such as Koo *et al.*, (2008) is that in their work no quantitative effect of angle is reported. In this work we investigated influences of inlet pressure, inlet temperature and nozzle divergent angle with the step changes in value.

### **3. Experimental**

In this work nozzle geometry and operating conditions of Binnie and Green has been used to validate the model. They represented nozzle dimension based on x-y coordinate system. Convergent-divergent angles of 30° and 15° have been applied for design of nozzle, respectively. The temperature in the range of 284-426 K and the pressure of 0.65-0.95 bar are operating conditions used by Binnie and Green, (1942).

### **4. Model development**

The governing equations used for analysis are the one-dimensional gas dynamic equations. Three conservation equations of the continuity, momentum and energy are incorporated with the equation of state of the gas. An ideal gas mixture is assumed, so apparent specific heats and gas constant are the weighted averages based on mole- fractions. Particle velocity is assumed to be the same as the local flow velocity, so a phase change does not cause any change in the momentum equation. The latent heat released during phase change is considered a heat generation source for the gas phase, and the difference in specific heats between the gas phase and the condensed phase is accounted for in the energy equation. The governing equations for a steady one-dimensional compressible flow are summarized in the next section. The generated particles remain inside the flow domain. The phase change reaction is assumed to be instantaneous, so diffusion or transport effects are not considered (Hill *et al.*, 1963; Kremmer & Okurounmu, 1965).

#### **4.1 Isentropic expansion**

Prior to starting of condensation, the flow through the nozzle is considered as one-dimensional, steady and isentropic.

Prior to the entrance of the nozzle, steam is at its stagnation condition, i.e.:

$$P=P_0, T=T_0, V=V_0=0 \quad (1)$$

The cross-sectional area at any place  $x$  or  $A=f(x)$  is given by geometric design of the nozzle. From this  $A=f(x)$ , the unknown properties  $P, T, V=f(A)$  or  $f(x)$  at any point  $x$  along the nozzle, can be calculated. The following assumptions were made to model the system, (i) flow is one-dimensional and steady-state. (ii) there is no heat transfer from the surrounding walls, and (iii) no frictions at the wall surfaces was considered.

Equations (3) to (6) are derived from Equation (2) using Leibniz's integral rule (see Equation (28) (Abramowitz & Stegun, 1972) for obtained liquid mixture ratio,  $\mu$ , along the nozzle. Further information about derivation was described in Appendix A.

$$\mu(x) = \frac{1}{\dot{m}} \int_{\eta=0}^{\eta=x} \rho_l \cdot I \cdot A(\eta) \cdot d\eta \frac{4\pi}{3} \left( r_0(\eta) + \int_{\eta_1=\eta}^{\eta_2=x} \frac{dr}{d\eta_1} d\eta_1 \right)^3 \quad (2)$$

$$\frac{dZ_1}{dx} = I \cdot A(x) \cdot 8\pi \quad (3)$$

$$\frac{dZ}{dx} = Z_1 \frac{dr}{dx} + I \cdot A(x) \cdot 8\pi \cdot r_0(x) \quad (4)$$

$$\frac{dS}{dx} = Z \frac{dr}{dx} + I \cdot A(x) \cdot 4\pi \cdot r_0^2(x) \quad (5)$$

$$\frac{d\mu}{dx} = \frac{\rho_L}{\dot{m}} S \frac{dr}{dx} + \frac{\rho_L}{\dot{m}} I \cdot A(x) \cdot \frac{4\pi}{3} \cdot r_0^3 \quad (6)$$

By rearranging the mass, momentum and energy equations, Equations (7) to (9) are obtained. Equation (10) shows particle diameter growth along the nozzle that should be calculated using droplet temperature,  $T_D$ . The droplet temperature has been calculated from Equation (14). Equation (13) is solved iteratively starting with a first guess  $T_D=T$  (Hill *et al.*, 1963; Kremmer & Okurounmu, 1965). Equations (11), (13) and (15) are used to calculate nucleation rate  $I$ , critical drop radius,  $r_0$ , and the average drop radius,  $r_{av}$ , respectively.

$$\frac{dP}{dx} = P \cdot \frac{KM^2}{M^2-1} \left[ \left( \lambda - \frac{1}{1-\mu} \right) \frac{d\mu}{dx} - \frac{1}{A} \frac{dA}{dx} \right] \quad (7)$$

$$\frac{dV}{dx} = -\frac{V}{KM^2} \cdot \frac{1}{P} \frac{dP}{dx} \quad (8)$$

$$\frac{dT}{dx} = T \cdot \frac{K-1}{K} \cdot \frac{1}{P} \frac{dP}{dx} + \lambda \frac{d\mu}{dx} \cdot T \quad (9)$$

$$\frac{dr}{dx} = \frac{3P}{2V \cdot U_{fg} \cdot \rho_L \cdot \sqrt{2\pi RT}} \cdot [RT_D - RT] \quad (10)$$

where  $I$ ,  $r^*$ ,  $r_0$ ,  $T_D$ ,  $r_{av}$  are determined from Equations (11), (12), (13), (14) and (15), respectively.

$$I = \left(\frac{P}{kT}\right)^2 \cdot v \cdot \sqrt{\frac{2\sigma}{\pi m}} \cdot e^{-\frac{4\pi\sigma(r^*)^2}{3kT}} \quad (11)$$

$$r^* = \frac{2 \cdot \sigma}{\rho_L \cdot RT \cdot \ln\left(\frac{P}{P_{s\infty}}\right)} \quad (12)$$

$$r_0 \approx 1.3r^* = \frac{2.6 \cdot \sigma}{\rho_L \cdot RT \cdot \ln\left(\frac{P}{P_{s\infty}}\right)} \quad (13)$$

$$\frac{2}{3} \frac{U_{fg}}{RT} \xi \left[ 1 - \frac{P_{s\infty}}{P} \exp\left(\frac{2\sigma}{\rho_L \cdot RT_D \cdot r_{av}}\right) \cdot \sqrt{\frac{T}{T_D}} \right] = \frac{T_D}{T} - 1 \quad (14)$$

$$r_{av} = \frac{3\dot{m} \cdot \mu}{\rho_L \cdot S} \quad (15)$$

All properties such as  $u_{fg}$ ,  $\sigma$ ,  $\rho_L$  and  $P_{S\infty,drop}$  are function of  $T_D$ . Internal energy,  $u_{fg}$ ; surface tension,  $\sigma$ ; liquid density;  $\rho_L$ , and saturated pressure;  $P_{S\infty,drop}$ , are calculated using Equations (16), (17), (18) and (19) (Smith *et al.*, 2005; Vargaftik *et al.*, 1983).

$$u_{fg} = h_{fg} + P \left( \frac{1}{\rho_g} + \frac{1}{\rho_l} \right) \quad (16)$$

$$\sigma = 235.8 \times 10^{-3} \left[ \frac{647.15 - T}{647.15} \right]^{1.256} \times \left[ 1 - 0.625 \frac{(647.15 - T)}{647.15} \right] \quad (17)$$

$$\rho_L = -2.9 \times 10^{-3} \times T^2 + 1.4483 \times T + 8.2191 \times 10^2 \quad (18)$$

$$P_{sat} = 1000 \times \exp\left( 16.3872 - \frac{3885.7}{T - 42.98} \right) \quad (19)$$

$$\rho_g = \frac{P}{RT} \quad (20)$$

$$h_{fg} = 3.17413 \times 10^6 - 2.45163 \times 10^3 \times T \quad (21)$$



## 4.2 Boundary conditions

To start the calculations in MATLAB, boundary conditions are necessary for each run. First of all Mach should be calculated using Equation (22). Then, Equations (23), (24) and (25) are used to obtain pressure, temperature and velocity, respectively (Kremmer & Okurounmu, 1965). The mass flow rate is calculated using Equation 26. Importance of mass flow rate is to avoid choking within throat point of the nozzle. For this reason, mass flow rate should be calculated precisely for each run. Other variables of  $Z_l$ ,  $Z$ ,  $S$  and  $\mu$  are considered zero in initial.

$$\frac{A}{A^*} = \frac{1}{M} \left[ \frac{2 + (K-1)M^2}{K+1} \right]^{\frac{K+1}{2K-2}} \quad (22)$$

$$\frac{P}{P_0} = \left[ 1 + \frac{K-1}{2} M^2 \right]^{\frac{K}{K-1}} \quad (23)$$

$$\frac{T}{T_0} = \left[ 1 + \frac{K-1}{2} M^2 \right]^{-1} \quad (24)$$

$$V = M \cdot \sqrt{kRT} \quad (25)$$

$$\dot{m} = A^* \cdot \psi_{\max} \cdot P_0 \cdot \sqrt{\frac{2}{RT_0}} \quad (26)$$

$$\psi_{\max} = \left( \frac{2}{K+1} \right)^{\frac{1}{K-1}} \cdot \sqrt{\frac{K}{K+1}} \quad (27)$$

## 5. Computational method

The calculations were carried out using numerical integration with the third-order Runge-Kutta integration method using MATLAB 2012. All equations of continuity, momentum, energy, nucleation and condensation were solved simultaneously. Finally, average drop radius obtained from Equation (15). The average drop radius is the most sensitive parameter calculated which is independent of the step size. Whatever considered small step size, consequently, results will have more accuracy. Step size less than  $10^{-5}$  is considered to be appropriate for this modeling and it can adjust step size automatically.

## 6. Results and discussion

Effects of divergent angle, inlet pressure and temperature on the droplet size have been investigated. Model results are validated using experimental data obtained by Hill *et al.* (1963). In Fig.1, the average drop radius and percentage of moisture,  $\mu$ , of model are compared with the experimental data.  $A/A^*$  is the ratio of area to the throat area. Model has predicted the average drop radius of 3.5 nm at length of 12 cm while the experimental data shows the size of 5.5 nm at the same point. The reason that experimental data shows the greater size than the model is due to the fact that effects of coagulation, agglomeration and wall heat transfer have been neglected in the modeling. Also, another reason can be in use of CNT as model of growth. Based on information in literature (Sinha *et al.*, 2009) there are other model of growth can be substitute instead of CNT model. It is not clear why the experimental results (Hill *et al.*, 1963) have not measured size of drop at length of 21cm possibly due to experimental limitation. At length of 12 cm the maximum error between experimental data and the model is 57%, but the error can surge to 30% at the end of nozzle. The percentage of moisture formation,  $\mu$ , also has a very good agreement with the available experimental data with the average error of 2%. There is no experimental data after 12 cm from inlet of the nozzle. Therefore, for other operating conditions which experimental data are not available; the experimental data were predicted using extrapolation of the modeling results.

Fig. 1: Comparison of the model results with experimental data obtained by Hill's *et al.* (1963).

### 6.1 Effect of divergent angle on the average drop radius

The average drop radius has been predicted at the end of the nozzle by applying different angles of 15°, 35°, 55°, and 75°. Fig. 1 shows effect of the nozzle angle at the constant pressure of 0.64 bar and temperature of 381 K on the drop radius along the length of nozzle.

For all divergent angles the drop radius is obviously increasing. Results prove that only for the divergent angle of 15° there is a marked improvement in average drop radius of 4.2 nm at the end of nozzle. However, trends of 35°, 55° and 75° are increasing at the beginning, then they suddenly fell back again by 1.5, 1 and 0.8 nm, respectively. The reason for this change is related to the sharp plunge in pressure and temperature values that have effects on supersaturation. Therefore, the critical radius and nucleation rate of drops are sensitive to the

supersaturation value (Koo *et al.*, 2008). In other word, the pressure has a direct effect on the drop radius. Accordingly, if the pressure reduces it will cause decrease in the supersaturation value. If the superasaturation value fell back till reach to the unity, it means that the nuclei's radius is very small and almost near to critical radius and probably the new nuclei will be evaporated back to the gas phase almost instantly. Exploited results confirm that an increase in the divergent angle resulting reducing drop radius. Only 20° increment in slope from 35° to 15° can increase drop size of condensate by 1.8 times more. This can be further explained using the results in Fig. 3 which shows that the pressure plummeted rapidly in divergent angle of 35°.

**Fig. 2: Effect of nozzle divergent angle on the average droplet radius.**

The pressure and temperature trends are obviously downward for all four divergent angles during expansion process presented in Fig. 3 and Fig. 4 Fig. 4, respectively. These have been obtained at the inlet pressure and temperature of 0.64 and 381 K, respectively. The pressure and temperature trends are followed by a period of stability hovered around the 5 cm from the inlet of nozzle. This point is mentioned as throat and velocity be equal to speed of sound or (M=1). The pressure and temperature, however, prove very erratic again, but the trends are downward after the throat.

**Fig. 3: Pressure profile of four different divergent angles of 15°, 35°, 55° and 75°.**

Once condensation starts, however, the process is fairly rapid and occurs over a relatively short distance. This region of condensation is termed the condensation shock (Oosthuizen & Carscallen, 1997). The process through the shock is represented by bounce back for the pressure and temperature trends at length of around 7 cm. The recovery is short-lived, however, the trends fall back again.

**Fig. 4: Temperature profile of four different divergent angles of 15°, 35°, 55° and 75°.**

To reach to coarse size of drops, the nozzle with the angle of 15°, which is compatible with Binnie and Green's work (Binnie & Green, 1942), has been taken for further investigation.

### ***6.2 Effect of inlet pressure on the average drop radius***

Fig. 5 shows the effect of inlet pressure on the drop radius. As discussed before pressure has a direct effect on the average drop radius. By an increase in pressure value the drop radius has been increased. Only 0.18 bar increment in pressure, the drop radius is increased by 60% at the end of nozzle (see Fig. 5). Average droplet size varies from 4 to 8 nm by increasing pressure from 0.64 to 0.95 bar in constant temperature of 383 K.

Fig. 5: Effect of inlet pressure on average droplet radius

### ***6.3 Effect of the inlet temperature on the average drop radius***

Fig. 6 shows influence of inlet temperature on the average drop size at the constant pressure of 0.64 bar. The temperature has an inverse effect on the average drop radius. As the temperature is increased, the average drop radius is reduced. The temperature has an effect on saturated pressure leading to increase in supersaturation value. Model has predicted only -10°C increment in temperature from 383 K to 393 K causes 30% increase in the average drop radius. Average droplet radius is increased from 3.5 to 5.2 nm by reducing the temperature from 393 to 373 K.

Fig. 6: Effect of inlet temperature on the average droplet radius

## **7. Conclusion**

A numerical model based on classical nucleation and growth was developed to calculate the nucleation and condensation of water vapor during rapid expansion in the Laval nozzle. The simulation results were validated with the experimental data by Hill's *et al.* (1942). In the range of conditions studied, the model has predicted that more than 90% of the condensation is due to growth of particles nucleated during an initial high nucleation rate stage. At the end of the nozzle, average drop size depends on nucleation rate. Influence of nozzle geometry and different process conditions on the average drop size has been studied. Nozzle divergent angle has a major effect on the drop radius. Only 20 degree deviation in divergent angle leads to change in effluent's average drop radius by 1.8 times. The model has predicted that an increase in inlet pressure causes increase in the average drop size, opposite to the effect of temperature. By increasing 0.18bar increment at inlet pressure, the average drop radius in

effluent stream increases up to 60%. Temperature has an inverse effect on the drop radius. Only 10° decrease in temperature from 393 K to 383 K cause 30% increase in average drop radius.

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| <b>Nomenclature</b> |   |   |  |
|---------------------|---|---|--|
| <b>Symbol</b>       | <b>Meaning</b>                                | <b>Unit (SI)</b>                                      |  |
| $A$                 | Cross section area                            | $m^2$   |  |
| $A^*$               | Throat area                                   | $m^2$   |  |
| $c_p$               | Specific heat at constant pressure            | J/kg.K  |  |
| $c_v$               | Specific heat at constant volume              | J/kg.K  |  |
| $h_{fg}$            | Enthalpy change due to condensation           | J   |  |
| $I$                 | Nucleation rate per unit volume               | nuclei/ $m^3 \cdot s$                                 |  |
| $K$                 | Isentropic expansion exponent                 | 1.3345  |  |
| $M$                 | Mach no.                                      | dimensionless   |  |
| $P$                 | Pressure                                      | $N/m^2$   |  |
| $P_{s\infty}$       | Saturation pressure                           | dimensionless   |  |
| $R$                 | Universal gas constant                        | 8.314 J/mol.K   |  |
| $S$                 | Differential parameter                        | dimensionless   |  |
| $T$                 | Temperature                                   | K   |  |
| $T_D$               | Drop temperature                              | K   |  |
| $u_{fg}$            | Change of internal energy due to condensation | J   |  |
| $V$                 | Velocity                                      | m/s   |  |
| $Z$                 | Variable generated using Leibnitz's rule      | nuclei/s  |  |
| $Z_l$               | Variable generated using Leibnitz's rule      | nuclei/m. s   |  |
| $k$                 | Boltzmann's molecular gas constant            | $1.3806488 \times 10^{-23} m^2 \cdot kg/ s^2 \cdot K$ |  |
| $\dot{m}$           | Mass flow                                     | kg/s  |  |

|                      |                                       |               |  |
|----------------------|---------------------------------------|---------------|--|
| $r$                  | Drop radius                           | m             |  |
| $r_0$                | Radius of smallest, newly-build drops | m             |  |
| $r_{av}$             | Average drop radius                   | m             |  |
| $r^*$                | Critical drop radius                  | m             |  |
| $x$                  | Length of nozzle                      | m             |  |
| <b>Greek symbols</b> |                                       |               |  |
| $\delta$             | Length of boundary layer              | m             |  |
| $\mu$                | Liquid-mixture mass ratio             | dimensionless |  |
| $\nu$                | Atomic or molecular volume            | $m^3$         |  |
| $\xi$                | Condensation coefficient              | 0.35          |  |
| $\pi$                | Mathematical constant                 | 3.14          |  |
| $\rho_L$             | Liquid density                        | $kg/m^3$      |  |
| $\sigma$             | Surface tension                       | N/m           |  |
| $\psi$               | Mass flow rate coefficient            | dimensionless |  |

## Appendix A

### The liquid part $\mu$ and its derivation

The liquid-mixture mass ratio ( $\mu$ ) is calculated along the length of nozzle ( $x$ ) considering the following assumptions, based on Kremmer *et al.* (1965):

- 1) The small droplets (nuclei) of radius  $r_0$  have been built on a nucleation rate  $I=f(p,T)$  in the past length along the nozzle ( $0 \rightarrow \eta \rightarrow x$ ).
- 2) Those nuclei grew, and their radius  $r$  was increased by  $\partial r/\partial x = f(p,T)$  steadily from the point where they were built  $\xi_1$  to the point  $x$  ( $\eta_1 \rightarrow \eta \rightarrow x$ ).

In this simulation, we assume all droplets grow at the same rate of  $\partial r/\partial x \approx dr/dx$ .

The  $\mu$  used to be defined along the length of the nozzle, and for this reason we have used  $\eta$  and  $\eta_1$  as dummy variables

Fig. 7: Expression of condensation ( $\mu$ ) at the length of nozzle.

By defining the control volume in the nozzle, the liquid mixture ratio was calculated using Equation (3). This equation includes two terms that are added to each other: one is the particles that are created at the beginning of control volume (at point of  $x=0$ ) and keep growing along the nozzle and another is particles that are created after point  $x=0$  and keep growing along the nozzle (Kremmer & Okurounmu, 1965).

|   |      |
|---|------|
| $\frac{\partial}{\partial z} \int_{a(z)}^{b(z)} f(x, z) dx = \int_{a(z)}^{b(z)} \frac{\partial f(x, z)}{\partial z} dx + f(b(z), z) \frac{\partial b(z)}{\partial z} + f(a(z), z) \frac{\partial a(z)}{\partial z}$ | (28) |
|---|------|

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