

# Condensation of flowing steam with binary nucleation of NaCl and water

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## Abstract

The effects of chemistry on the flowing steam nucleation are in particular unexplained. An approach is used in the paper which is based on binary nucleation of main impurity NaCl and water. Physical and mathematical models are described and are applied on the steam flow with condensation in convergent-divergent nozzle. Binary nucleation numerical model is applied for the calculation of the flow with condensation in nozzle with expansion rate in divergent nozzle part  $\bar{P} = 4\,500\text{ s}^{-1}$ . The flow in the nozzle is smooth and it is possible to observe only a small delay of the pressure and a small shock of the temperature downstream of the nozzle throat. © 2007 University of West Bohemia. All rights reserved.

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## 1. Introduction

The flow of water steam with condensation is still an open problem that faces us. It has great importance especially in the flow through condensing steam turbines. The effects of chemistry on the steam nucleation are in particular unexplained.

The effects of chemical impurities on nucleation and following condensation can occur mainly in Salt Solution Zone (SSZ). In the past a mathematical model and code were developed [7], [8] that simplified the process and took in account the nucleation in SSZ by impulsive nucleation on the low SSZ boundary - steam saturation line (SSL).

More complicated approach is used in the paper which is based on binary nucleation of main impurity NaCl and water. Physical and mathematical models are described and are applied on the steam flow with condensation in convergent-divergent nozzle.

## 2. Steam expansion in phase transition zone

A nucleation of two types can occur in the water steam flowing in a nozzle or in a turbine: homogeneous (spontaneous) and heterogeneous. The homogeneous nucleation occurs during the expansion of pure water steam under the steam saturation line with a delay at a sufficient subcooling. This is followed by the growth of droplets caused by condensation. The heterogeneous or binary nucleation can occur already in SSZ, above SSL, on the chemical impurity contained in the superheated water steam.

Superheated water steam, expanding in the steam turbine stages, contains impurities of various kinds. From the point of heterogeneous nucleation view, it is possible to divide these impurities into two categories.

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The solid particles insoluble in water and in the water steam form the first category. Concentration of these solid impurities in the steam is most probably too small to affect in any significant degree by the heterogeneous nucleation the homogeneous nucleation.

Water and water steam soluble chemicals form the second category. These chemicals can be partly dissolved in the superheated steam and they can be present also in a form of molecule clusters. Numerous inorganic and organic chemicals exist in the second category. They are impurities in the superheated steam inside the steam turbines or nozzles - see Bellows [2] - e.g.: NaCl, Na<sub>2</sub>SO<sub>4</sub>, Sodium acetate etc. We shall further consider NaCl; a chemical, which is most often present in the water-steam and the properties of which have been most researched.

Fig. 1 shows expansion of the water-steam, containing chemical impurity NaCl, with binary nucleation in the phase transition zone and for comparison also expansion of pure water-steam.

The expansion in phase 1 first reaches the solution saturation line of the NaCl in the water, called three-phase boundary (TPB). This is at the top limit of the SSZ. The binary nucleation of the water molecules around the molecules or on clusters of molecules of NaCl, can start under this line.

The expansion goes through the SSZ in phase 2. Binary nucleation is a dynamic process and needs some subcooling under TPB. The process of binary nucleation 3 can start and continues even under the steam saturation line. A condensation occurs on nucleation embryos and continues in phase 4 until the wet steam reaches the final state at the nozzle outlet.

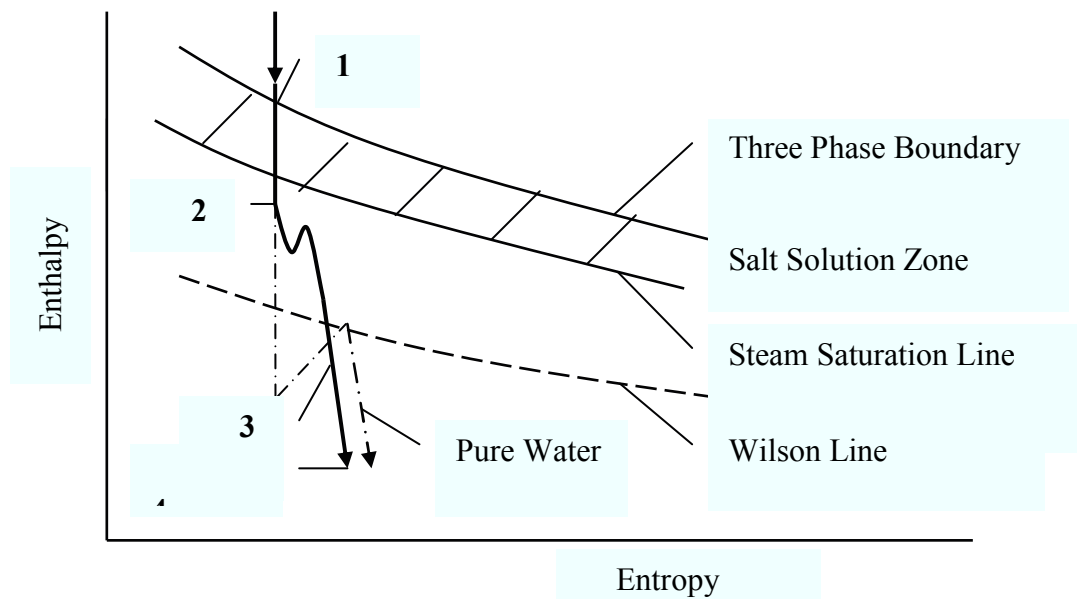


Fig. 1. Steam expansion line with binary nucleation in phase transition zone.

### 3. Computational Model and its Application

A two-dimensional wet steam flow is described by the system of Euler equations. The system is linked with equations describing binary nucleation and with equations describing growth of water droplets by condensation.

The mathematical model of the binary nucleation is based on the Becker-Doering relationship [1] for the nucleation rate  $\underline{J}$  [ $\text{m}^{-3}\text{s}^{-1}$ ] for pure water steam:

$$J = \alpha_K \frac{\sqrt{2\sigma N_1^3 \pi^{-1}}}{(RT_1)^2 \rho_2} p_1^2 \cdot \exp\left(\frac{-K_G \Delta G^*}{kT_1}\right), \quad (1)$$

where 
$$\Delta G^* = \frac{16\pi\sigma^3}{3(\rho_2 RT_1 \ln S)^2}.$$

The Becker-Doering theoretical formula (1) is corrected by empirical parameters - the condensation coefficient  $\alpha_K = 1.00$  and Gibbs free energy  $\underline{\Delta G}^*$  correction factor  $K_G = 1.30$ . Values of these parameters were fitted to experimental results gained with pure water steam in the shock tube – see Lankaš [6].  $\underline{N}_1$  [ $\text{kg}^{-1}$ ] is number of  $\text{H}_2\text{O}$  molecules and  $\underline{k}$  is the Boltzmann constant. Index  $\underline{1}$  is for steam and  $\underline{2}$  for water.

Kelvin formula is used for critical radius  $\underline{r}^*$  calculations of the embryos:

$$r^* = \frac{2\sigma}{\rho_2 RT_1 \ln S}. \quad (2)$$

On the contrary to the spontaneous nucleation of pure water steam [7] there are performed in the relationships some changes.

Super saturation  $\underline{S}$  is defined as follows:

$$S = \frac{p}{p_{sNaCl}} \cdot \frac{1}{a_{wNaCl}}, \quad (3)$$

where  $\underline{p}_{sNaCl}$  is the saturation pressure at TPB and  $\underline{a}_{wNaCl} = 0.71668$  is the activity coefficient for water and NaCl.

Surface tension  $\underline{\sigma}$  is defined for saturated water solution of NaCl and in the embryo is described by empirical function of temperature  $\underline{T}$  [K]:

$$\sigma_{NaCl} [\text{N/m}] = (86.43 - 0.1674(T - 273.15))10^{-3}. \quad (4)$$

Data for  $\underline{a}_{wNaCl}$  and  $\underline{\sigma}_{NaCl}$  were created on the base of Gorbunov and Hamilton [4] publication.

For saturation pressure  $\underline{p}_{sNaCl}$  at TPB and low pressures (0.5-2.0 bar) was created also an empirical function of temperature  $\underline{T}$  [K]:

$$\text{Log}_{10} p_{sNaCl} [\text{bar}] = 5.4763 - 2092,69/T. \quad (5)$$

The system is linked with equations describing growth of heterogeneous droplets by water condensation starting from critical radius of droplets. The relation of Gyarmathy [5] is used:

$$\frac{dr}{dt} = \frac{\lambda \Delta T}{L \rho_2 (1 + 3.18 K_n)} \cdot \frac{r - r^*}{r^2}, \quad (6)$$

where  $\underline{t}$  is time,  $\underline{\lambda}$  is thermal conductivity of steam,  $\underline{L}$  is latent heat and  $K_n$  is Knudsen number.

It is assumed that the model will be used only for small total wetness ( $y < 0.06 \text{ kg.kg}^{-1}$ ), and that the steam phase can be considered as an ideal gas at low pressures. It is also assumed that there is no slip between the steam phase and the droplets.

The Finite-volume method is used for the solution of the system of equations. The 2D domain is discretised by unstructured triangular mesh. This mesh is locally refined especially in area of the binary nucleation zone. The number of triangles is from 10 000 to 100 000. A hybrid explicit TVD/up-wind scheme is used to solve the problem numerically.

### 3.1. 2D Nozzle and Flow Mode

Binary nucleation numerical model was applied for the calculation of the flow with condensation in nozzle with expansion rate in divergent nozzle part  $\ddot{P} = 4\,500\text{ s}^{-1}$ . The same nozzle was used in experiments performed at CTU [3]. The shape of the nozzle is obvious from the enclosed figures. The throat of nozzle is 0.048 m. The selected total inlet parameters are:  $P_{at} = 2.75\text{ bar}$ ,  $T_{at} = 428.15\text{ K}$ . The flow in the nozzle is transonic and steam condensation occurs.

### 3.2. Calculation Results and Discussion

The expansion of the steam in the nozzle can be evaluated according to the contours of Mach number in Fig. 2. The velocity of flow in the nozzle passage gradually grows and the sonic velocity ( $M = 1$ ) is reached in the proximity of the nozzle throat. Downstream of the throat, the flow is overall supersonic. A small irregularity in Mach number contours is noticeable behind the nozzle throat. Shock waves are located downstream of the divergent nozzle part.

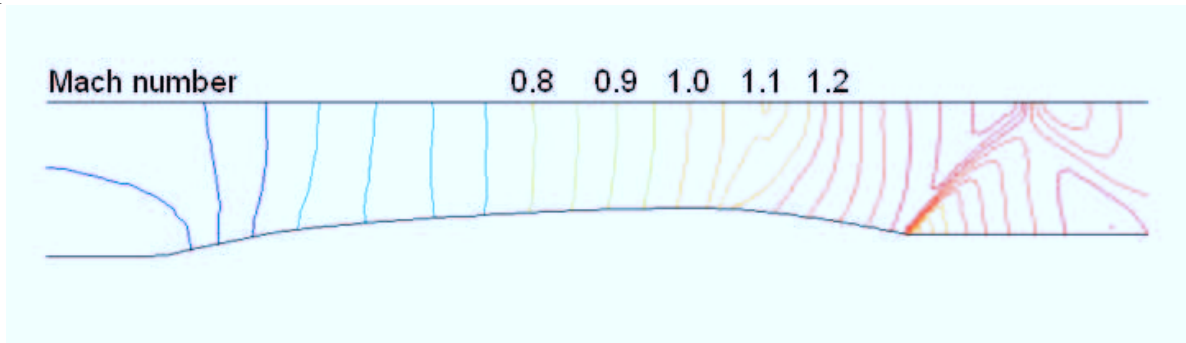


Fig. 2. Mach number contours in the nozzle.

Fig.3 shows pressure and temperature distributions along the straight wall of the nozzle. It is possible to observe a small delay of the pressure and a small shock of the temperature downstream of the throat. They are connected with the final part of binary nucleation zone.

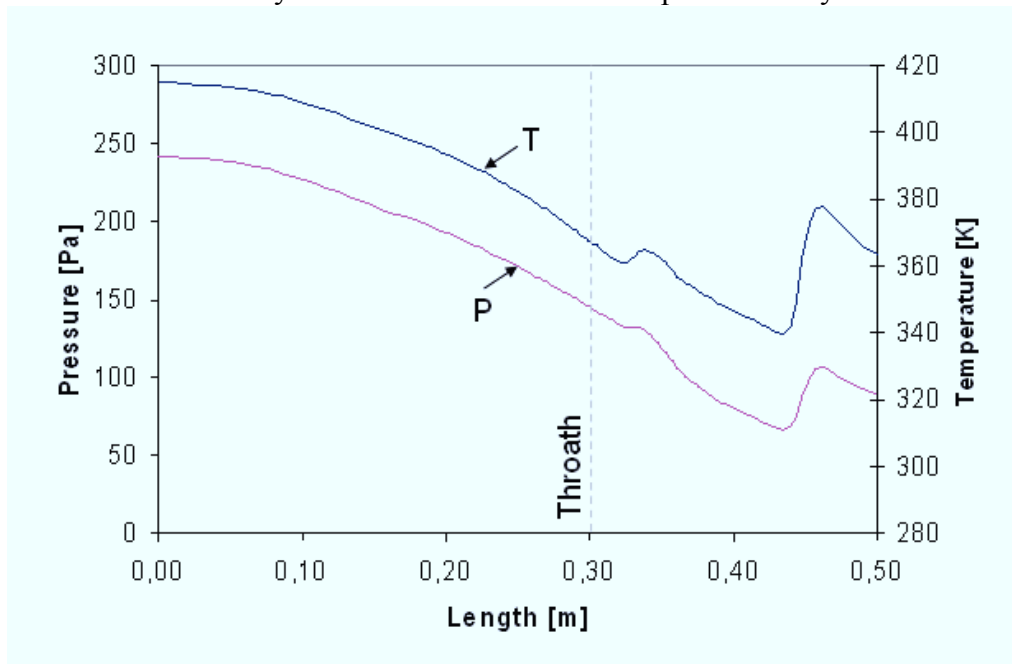


Fig. 3. Pressure and temperature distributions along the straight wall of the nozzle.

The zone of the binary nucleation is noticeable in Fig.4 showing the distribution of the binary nucleation rate in the form of Log J contours.

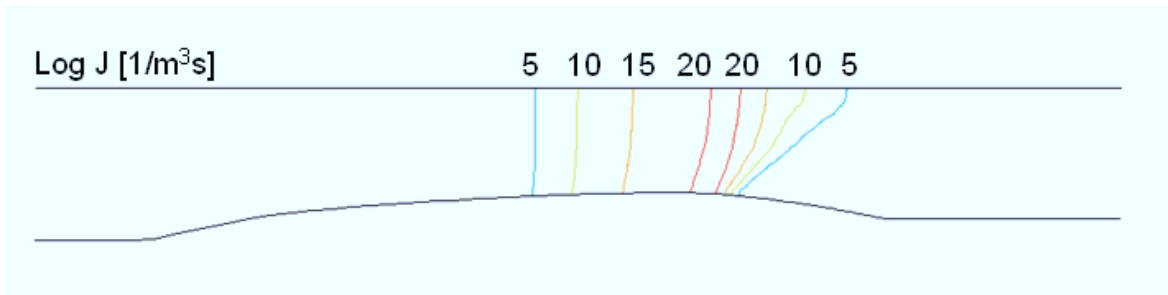


Fig. 4. Binary nucleation rate ( $\text{Log } J[\text{Nm}^{-3}\text{s}^{-1}]$ ) in the nozzle.

The onset of the binary nucleation is located in the convergent part of the nozzle and it is finished downstream of the throat. The zone of binary nucleation is wide.

Fig.5 shows the courses of some nucleation and condensation parameters along the straight wall of the nozzle. Position of the SSZ zone is allocated between zero values of the subcooling course under TPB and subcooling course under SSL.

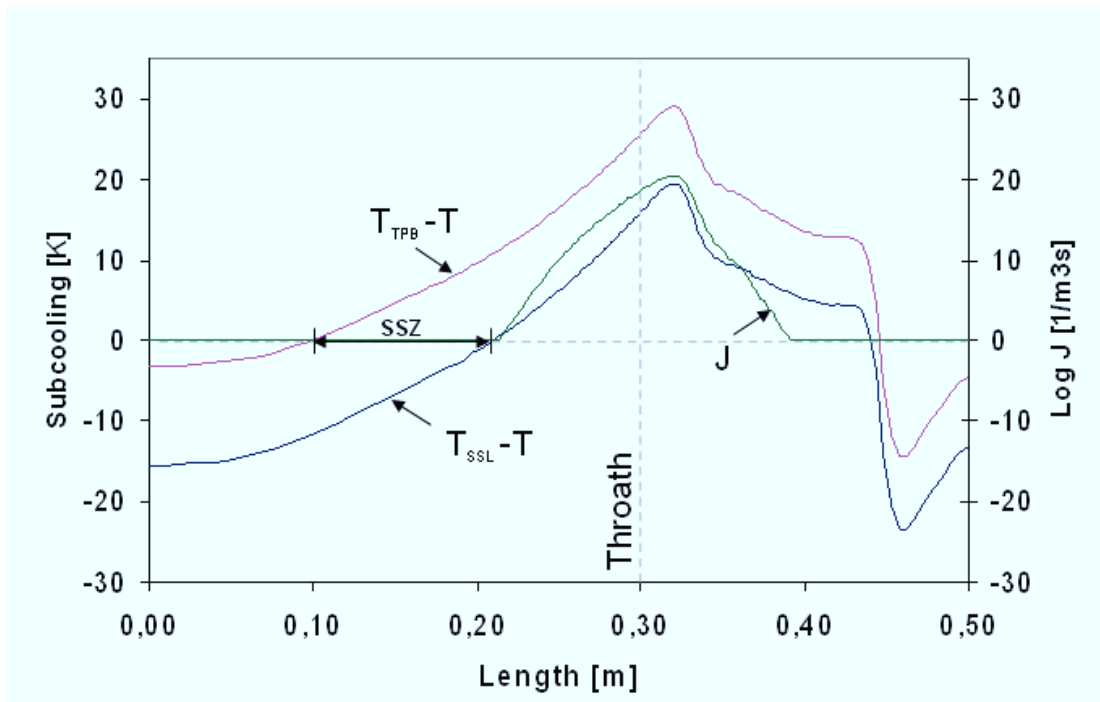


Fig. 5. Binary nucleation rate  $J$ , subcooling under TPB ( $T_{\text{TPB}} - T$ ), subcooling under SSL ( $T_{\text{SSL}} - T$ ) along the nozzle straight wall.

The zone of binary nucleation is visualised by the course of nucleation rate in form of Log J. Binary nucleation starts at the subcooling under TPB ( $T_{\text{TPB}} - T$ ) = 11 K and subcooling under SSL ( $T_{\text{SSL}} - T$ ) = 1 K. Downstream of the starting point a fast subcooling under TPB ( $T_{\text{TPB}} - T$ ) of the steam occurs with maximum value of  $(T_{\text{TPB}} - T)_{\text{max}} = 29$  K. The subcooling under SSL ( $T_{\text{SSL}} - T$ ) has maximum value  $(T_{\text{SSL}} - T)_{\text{max}} = 19$  K. In the rear part of the nozzle subcooling decreases in direction to the outlet reaching the values  $(T_{\text{TPB}} - T) = 13$  K and  $(T_{\text{SSL}} - T) = 4$  K.

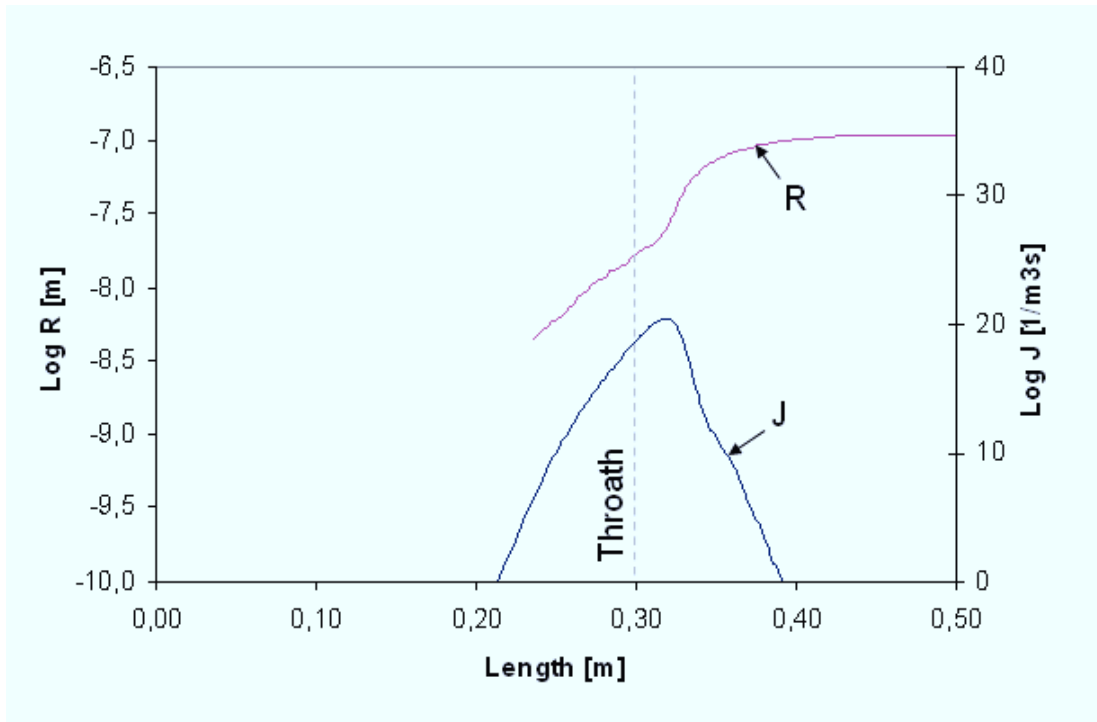


Fig. 6. Heterogeneous droplet radius  $R_{Het}$ , binary nucleation rate  $\underline{J}$  along the nozzle straight wall.

Fig.6 shows the calculated course of the droplet radius. Droplet sizes increase in the direction of nozzle outlet.

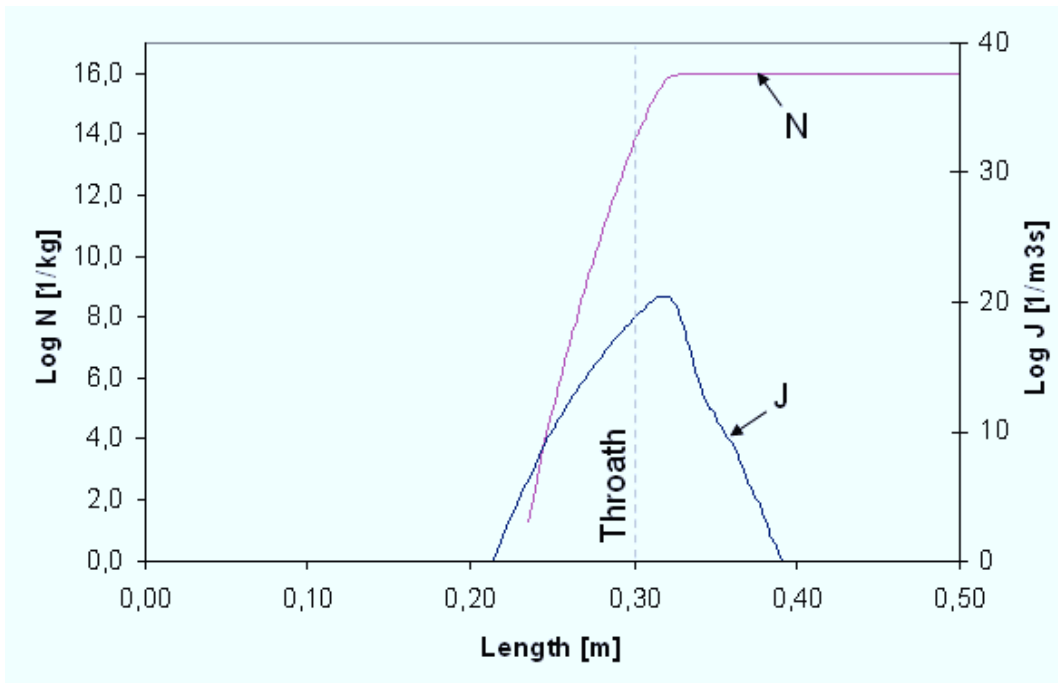


Fig. 7. Embryo number  $N_{Het}$ , binary nucleation rate  $\underline{J}$  along the nozzle straight wall.

In front of the nozzle outlet, the droplets originated by the binary nucleation reach mean size about  $R_{\text{Het}} = 1.0 \text{ e-}07 \text{ m}$ . It is noteworthy that the heterogeneous droplets grow quickly in the region close behind the nozzle throat, in the final part of the binary nucleation zone.

Embryo number produced in binary nucleation zone grows fluently to the maximum value at the end about  $N_{\text{Het}} = 1.0 \text{ e+}16 \text{ kg}^{-1}$  – see Fig.7.

#### 4. Conclusion

The effects of chemical impurities on nucleation and following condensation can occur mainly in Salt Solution Zone (SSZ).

Mathematical approach of describing the nucleation and condensation is used in the paper which is based on binary nucleation of main impurity NaCl and water with following water condensation.

Binary nucleation numerical model is applied for the calculation of the flow with condensation in nozzle with expansion rate in divergent nozzle part  $\ddot{P} = 4 \text{ 500 s}^{-1}$ . The flow in the nozzle is smooth and it is possible to observe only a small delay of the pressure and a small shock of the temperature downstream of the nozzle throat.

The zone of binary nucleation is wide. Binary nucleation starts at the subcooling under TPB ( $T_{\text{TPB}} - T = 11 \text{ K}$ ) and subcooling under SSL ( $T_{\text{SSL}} - T = 1 \text{ K}$ ). Downstream of the starting point a fast subcooling under TPB of the steam occurs with maximum value of  $(T_{\text{TPB}} - T)_{\text{max}} = 29 \text{ K}$ . The subcooling under SSL ( $T_{\text{SSL}} - T$ ) has maximum value  $(T_{\text{SSL}} - T)_{\text{max}} = 19 \text{ K}$ . In the rear part of the nozzle subcooling decreases in direction to the outlet reaching the values ( $T_{\text{TPB}} - T = 13 \text{ K}$  and  $(T_{\text{SSL}} - T) = 4 \text{ K}$ ).

In front of the nozzle outlet, the droplets originated by the binary nucleation reach mean size about  $R_{\text{Het}} = 1.0 \text{ e-}07$ .

Embryo number produced in binary nucleation zone grows fluently to the maximum value at the end about  $N_{\text{Het}} = 1.0 \text{ e+}16 \text{ kg}^{-1}$ . For such number of produced droplets it is necessary to be in the steam as minimum 1 ppb of NaCl.

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