Some peculiarities of superheated water flow in contracting-expanding nozzles and their influence on droplet dimension distribution in an atomized water plume

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Abstract. New calculation data on superheated metastable water flow in atomizing Laval type nozzles is presented. The calculating model is discussed on the assumption of predominating nucleation role in liquid atomization. The Mach number variation is presented for diffuser part of the nozzle taking into account the sound velocity variation in a vapor-liquid system. The new criterion, based upon experimental and calculating data, which determines the reaching of full-flashing regime, is proposed for contracting-expanding nozzles. The submicron mass fraction is considered to be a function of dimensionless parameter, which is the critical radius bubble surface tension energy ratio to chemical potential of phase transition for critical bubble radius at certain pressure drop.

1. Introduction.
The importance of finely atomized superheated water (and some other liquids) atomization in micron and submicron range of droplets is determined by great specific droplet surface area. It allows applying atomized superheated liquids for water injection in various gas turbine combined-cycle power units, for spray-cooling, for fuel injection and for new efficient fire-fighting and smoke-capturing technologies. The investigations of superheated liquids flows have been undertaken for a long time [1-2]. The flashing processes (“explosive boiling”) due to quick pressure fall were investigated as well. A shape of flashing plumes, their evolution and effect of inlet liquid parameters on the liquid atomization process, and, in some cases [3-4], droplet size dispersion were studied for short contracting nozzles. Publications are rather rare for contracting-expanding nozzles [5]. It is especially worth noting the work [6] with a very detailed description of modern attitude to explosive boiling of metastable liquid in the contracting nozzles and corresponding atomized water plums and with a discussion of some approaches to dimensionless treatment of results. The term “full flashing” widely used in that and some other works has to be defined more exactly. Usually it is understood as a liquid defragmentation level at which the maximum of the atomization plume angle (about 180°) is obtained at the outlet of the short contracting nozzle. It is admitted (and validated by photographs with 2 µm resolution) that liquid is atomized into droplets with diameter less than 5 µm. JIHT experiments [7-8] for short contracting nozzles have shown that droplet size distribution is more complicated even at large diverge plum angles [8]. Superheated water atomizing experiments with contracting-expanding nozzles were described in [9-10]. Results of present calculations refer to these experiments.
2. Short description of experimental conditions.
Droplet size distribution in atomized superheated water plume was studied at “Raspyl” plant [8-10]. In these experiments nozzles had relatively long (about 30 mm) diffuser part after contracting part and cylindrical throat. The divergence angle was about 12°. The throat diameter $d_0$ was 0.7 and 1.6 mm. In addition to measurement of initial parameters $P_0$, $T_0$ and water flow rate there were flow temperature and pressure measurements in several cross-sections along the diffuser part of the nozzle [11].

![Figure1. Calculating nozzle configuration.](image)

The flow characteristics (mass fraction distribution for micron and submicron droplet size) were determined by plume monochrome scattering level measurement at various angles (up to 45°) by a technique described in [12]. It is based on Mi theory, but for dense plumes of atomized superheated water it is important to take into account secondary multilateral scattering [13] especially at large angles. So measurement of integral laser ray attenuation at various angles was used for treating experimental data using the special technique of evaluation of multilateral scattering. The last experimental results are presented in [14].

3. The explosively boiling superheated metastable water flow. Theory and calculating evaluations.
The problem of explosively boiling superheated water flow in the nozzle of above geometry was under consideration. Mathematical model included the mass, impulse and energy conservation equations and nucleation equations in quasi stationary one-dimensional equilibrium approach. The flow rate was changing parametrically. The solution was reached in iteration process at corresponding boundary conditions (inlet pressure and temperature, outlet pressure).

Hydrodynamic equations (Euler stage):

$$\frac{\partial (F \cdot \rho \cdot u)}{\partial z} = 0 \quad (1)$$

$$\frac{\partial (F \cdot \rho \cdot u \cdot u)}{\partial z} = -F \cdot \frac{\partial P}{\partial z} - \Pi \cdot \tau \quad (2)$$

$$\frac{\partial (F \cdot \rho \cdot u \cdot h)}{\partial z} = -F \cdot u \cdot \frac{\partial P}{\partial z} \quad (3)$$

$$\Pi \cdot \tau = \frac{F \cdot \xi}{d_e} \quad ; \quad \xi \cdot (Re) = (1.82 \cdot \lg(Re) - 1.64)^{-2} \quad ; \quad d_e = \frac{4F}{\Pi} \quad (4)$$

$F$ is the nozzle cross-section square at $z$ coordinate along the nozzle; $\rho$ is the vapor-liquid mixture density; $u$ is the flow velocity; $z$ is the coordinate along the nozzle; $P$ is the pressure in vapor-liquid mixture; $\Pi$ is the nozzle cross section perimeter at $z$ coordinate; $\tau$ is the friction stress at nozzle wall;
$h$ is the vapor-liquid mix enthalpy; $Re$ is the Reynolds number and $d_e$ is the nozzle cross-section diameter.

Lagrange stage: heterogeneous nucleation equations at each time step:

$$H_N = \rho_l \left( \frac{N_d}{m} \right)^{3/2} \cdot \left( \frac{2\sigma}{\pi} \right)^{1/2} \exp \left( - \frac{W_{cg}}{k_B \cdot T_l} \right)$$ (5)

$$R_{cr} = \frac{2\sigma}{(P_{sat}(T_l) - P_l)}$$ (6)

$$W_c = \frac{16\pi \cdot \sigma^3}{3(P_{sat}(T_l) - P_l)^2} ; W_{cg} = G \cdot W_c$$ (7)

$$N_{bi} = \int_{t_i}^{t_{i+1}} H_N dt ; N_{bz} = \int_0^z N_{bi} dz$$ (8)

where $G$ is the heterogeneous factor.

Let us discuss an influence of heterogeneous factor upon nucleation process. Boiling is intensified due to volume heterogeneity (in our case it is gaseous bubbles release according to Henry law), i.e. because of surface heterogeneity. Surface heterogeneity means formation of initial vapor clusters on the surfaces with different roughness and wettability. There is a summary in [15] for volume heterogeneous factor dependence in nucleation process in nozzles upon liquid initial temperature for certain pressure drop range (10-200 GPa/s). In our case it is about 0.0015, which well corresponds to [15]. The same work gives expression for surface heterogeneous factor. In our case it is several orders less than the volume one (calculated per volume unit). Hence, it was not taken into account in this model.

The influence of heterogeneous factor upon nucleation rate needs deeper investigations. As a matter of fact the surface characteristics influence upon surface heterogeneity and some other peculiarities should be taken into account.

Vapor bubble growth is described by Relay-Lamb equation:

$$R \cdot \frac{d^2R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 = \frac{1}{\rho_l} \cdot \left( P_0 - P_l - \frac{2\sigma}{R} - \frac{4\mu_l}{R} \cdot \frac{dR}{dt} \right)$$ (9)

The following dimensionless variables give a possibility (according to [16]) to express the results of numerous calculation of Relay-Lamb equation in the following form (it practically coincides with Relay form at $t/t^* > 50$):

$$\xi = \frac{R}{R_0} ; \; t^* = R_0 \cdot \left( \frac{3\rho_l}{2\Delta P} \right)^{1/2}$$ (10)

In dimensional form it is:

$$R = t \cdot \left( \frac{2\Delta P}{3\rho_l} \right)^{1/2}$$ (11)

Sound velocity in vapor-liquid system (without phase transition) may be expressed as [17]:

$$C = \left\{ 1/ \left[ (\varphi \cdot \rho_l + (1-\varphi) \cdot \rho_v) \cdot \left( \frac{\varphi}{c_v^2 \cdot \rho_v} + \frac{1-\varphi}{c_l^2 \cdot \rho_l} \right) \right]^{1/2} \right\}$$ (12)

Here: $C$ is the sound velocity in the system vapor-liquid; $\varphi$ is the vapor volume fraction; $\rho_v$ is the vapor density; $\rho_l$ is the liquid density; $c_v$ is the sound velocity in vapor and $c_l$ is the sound velocity in liquid.
Thus the change of vapor volume fraction along the nozzle axis was obtained, taking into account the nucleation rate and the bubble growth dynamics. When vapor volume fraction reaches approximately 1.4, a qualitative system transformation takes place. A bubble containing liquid transforms into vapor-droplet system, and the foam disintegrates.

At the same time this process shouldn’t be understood as a boiling shock but it may be interpreted as a continuous density, rather quickly changing process in a quasi-homogenous system. At first it takes place because of nucleation and bubble growth and then (after foam disintegration) it occurs due to droplet evaporation.

The problem of foam disintegration is complicated by bubble diameter variation. In this model it is assumed that there is a certain statistical distribution for bubble diameter near critical bubble radius, which corresponds to maximum nucleation rate, taking into account the subsequent bubble growth. This assumption is possible because of explosive boiling character.

Herewith two principally different cases take place:
1. In the contracting part of the nozzle, pressure drops lower than saturation pressure (corresponding to initial temperature). The boiling begins in this part of the nozzle. The flow becomes compressible, and the sound velocity decreases dramatically. After the foam disintegration the vapor-droplet flow density falls in nozzle diffuser part due to droplet evaporation in supersonic flow; the sound velocity slowly grows, figures 10-11).
2. Pressure along the narrowing part of the nozzle exceeds saturation pressure everywhere, this is why the boiling is formally impossible in diffuser part of the nozzle according to conservation equation.

In this case, flow disintegration probably takes place just after the nozzle throat because of aerodynamic forces, and we are to assume the presence of pressure drop here (to pressure lower than saturation pressure). The value of this drop may be determined from experimental drop distribution and then it may be corrected in iteration process. The explosive boiling takes place in liquid fragments, and after this the flow becomes a vapor-droplet mixture. Herewith (as for short nozzles) the bimodal droplet size distribution may be expected due to two different processes of liquid defragmentation [17]. After foam defragmentation droplet evaporation (which leads to vapor-droplet mixture density change) was calculated using approximation [18] at each time step.

\[
j_{\text{max}} \approx 0.82 \cdot S \cdot \rho_v \cdot \frac{\sqrt{2 R_u \cdot T'}}{2 \cdot \sqrt{\pi}}
\]

where: \(j_{\text{max}}\) is the evaporating fluid mass flow, \(S\) is the inter-phase boundaries summary square; \(\rho_v\) is the vapor density; \(T'\) is the liquid phase temperature and \(R_u\) is the vapor gas constant.

**Figure 2.** Pressure distribution along the nozzle (\(T_{\text{in}}=240^\circ\text{C}, G=0.058\ \text{kg/s})

**Figure 3.** Density distribution along the nozzle (\(T_{\text{in}}=240^\circ\text{C}, G=0.058\ \text{kg/s})
Figures 2-7 represent parameters distribution (pressure, density, flow velocity, nucleation rate, mixture temperature along longitudinal nozzle axis corresponding to experimental conditions: flow rate $G=0.058$ kg/s; inlet pressure $P_i=4$ MPa; inlet temperature $T_{in}=513K$ and geometry – figure 1.

Figure 4. Flow velocity distribution along the nozzle ($T_{in}=240^\circ C$, $G=0.058$ kg/s).

Figure 5. Temperature distribution along the nozzle ($T_{in}=240^\circ C$, $G=0.058$ kg/s).

Figure 6. Nucleation rate distribution along the nozzle ($T_{in}=240^\circ C$, $G=0.058$ kg/s).

Figure 7. Mach number distribution along the nozzle ($T_{in}=240^\circ C$, $G=0.058$ kg/s).

Spray plumes in figure 8 illustrate the experimental validation of the explosive boiling point place on the longitude nozzle axis. There are the atomized superheated water plumes obtained by cutting the diffuser at certain longitudinal coordinates.
4. Dimensionless experimental and calculating data treatment.

As it was pointed out above, the pressure in contracting part of contracting-expanding nozzles may exceed saturation pressure (corresponding to inlet temperature $T_0$). It means that as for short nozzles we have (according to classification [5, 18]) the regime of outside disintegration characterized by influence of many factors: disintegration by aerodynamic forces, bar-capillary instability, explosive boiling in liquid fragments, and sound wave shocks. On the contrary, explosive boiling in contracting-expanding nozzles may develop more effectively. And from the certain liquid superheating point the liquid defragmentation process is fully controlled by explosive nucleation. The problem of dimensionless treatment is to determine the parameter which governs this conversion.

According to the hypothesis [5], the initial divergence angle of atomized superheated liquid at the outlet of the short conic nozzle at certain reached superheating level depends fully upon nucleation process characteristics. As for our interpretation, “full flashing atomization” should be understood (as it was mentioned above) as a reaching of practically monomodal submicron droplet size distribution.

Unlike dimensionless treatment of results which refer to one molecule [5] we are trying to analyze the problem as applied to a critical cluster (critical bubble radius). If the surface tension energy is divided by chemical potential energy of vapor mass in the volume of critical cluster ($R_{cr} = 2\sigma/\Delta P$) the following criteria may be obtained:

$$K_0 = \frac{\sigma \cdot 4\pi \cdot R_{cr}^2}{k_b \cdot T \cdot \ln(R_p) \cdot N_m}$$  \hspace{1cm} (14)

where

$$N_m = \frac{4\pi \cdot R_{cr}^3 \cdot \rho_v \cdot N_A}{3 \cdot M_t}$$  \hspace{1cm} (15)

$N_m$ is the number of molecules in the critical cluster.

Then:

$$K_s = \frac{\sigma \cdot 4\pi \cdot R_{cr}^2 \cdot 3M_t}{k_b \cdot T_{in} \cdot \ln(R_p) \cdot 4\pi \cdot R_{cr}^3 \cdot \rho_v \cdot N_A}$$  \hspace{1cm} (16)
Numerator and denominator of the previous expression multiplied by $P_{sat}$, taking into account:

$$R_p = \frac{P_{sat}}{P_1}; \quad R_{cr} = \frac{2\sigma}{(P_{sat} - P_1)}; \quad R_v \cdot T_{in} = \frac{k_b \cdot N_A}{M_t} = \frac{P_{sat}}{\rho_v}$$

(17)

give:

$$K_s = \frac{3(1 - 1/R_p)}{2\ln(R_p)}$$

(18)

Here: $R_{cr}$ is the critical bubble radius; $\rho_v$ is the vapor density at the temperature $T_{in}$; $N_A$ is the Avogadro number and $M_t$ is the molar mass.

Herewith independence of the criterion from surface tension is connected with various size of critical bubble radius for various liquids (14). It should be noted that the proposed criterion is quite correct as far the heterogeneous factor is constant (in this case it may be extracted from exponent in (5)) and its influence just changes the value of criterion at which “full flashing” regim occurs. Overwise it should be considered as an independent criterion.

The value $K_s = 1$ corresponds to $R_p \sim 3.5$ or $\sim 145^\circ C$. In the expression for this criterion, the radius of critical bubble is taken without Thompson correction factor. For our conditions overheating is about 25$^\circ C$. So inlet pressure should be adjusted correspondingly. This is why we can predict the beginning of nucleation process dominating in superheated water atomization at the temperature about 180$^\circ C$ and a good agreement with experimental results.

It is necessary to underline that the criterion $K_s$ is universal for various liquids, if one does not take into account the Thompson correction factor.

**Conclusion.**

1. The comparison of experimental and calculating results shows satisfactory agreement and reveals important peculiarities of thermo-physical and hydrodynamic processes in the flow of the superheated water in contracting-expanding nozzles which are connected with water explosive boiling. These processes determine the high level of atomization in spray plums.

2. The new criterion $K_s$, proposed in this article, describes well the transition to “full-flashing atomization” regime for contracting-expanding nozzles if heterogeneous factor is constant. Otherwise heterogeneous factor should be considered as an independent criterion.

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