Numerical Simulation of the Steam Flow with Condensation in a Nozzle

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The two-population numerical model of hetero-homogeneous condensation is used for the calculation of the wet steam flow with condensation in a convergent-divergent nozzle. This computational model applies governing equations of the wet steam flow and equations of spontaneous nucleation. Parallel heterogeneous nucleation is evaluated on the assumption that heterogeneous water droplets originate by nucleation on chemical impurity (NaCl) in Salt Solution Zone close above the steam saturation line. The calculation results of the flow in the nozzle with mean expansion rate $\dot{\bar{P}} = 4500\ s^{-1}$ in divergent nozzle part are described and the effects of heterogeneous and/or spontaneous nucleation and condensation are discussed and compared with experiment.

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 [1]. The effects of chemistry on the steam nucleation are in particular unexplained.

Convergent-divergent nozzles are suitable for research of processes running during the condensation of flowing water steam. Lot of significant experiments were performed with nozzle flow in the past. Experiments with the effects of various chemicals on the flow with condensation in convergent-divergent nozzle were performed in the frame of international project "Steam, Chemistry, and Corrosion in the Phase Transition Zone of Steam Turbines" [2]. Petr and Kolovratnik performed the experiments on the Czech Technical University (CTU) experimental facility in Prague, Czech Republic. The project was organized by EPRI, Palo Alto, USA.

This contribution connects on the experiments performed in the mentioned project. The two-population numerical model of hetero-homogeneous condensation [1] is used for the calculation of the steam flow with condensation in a convergent-divergent nozzle. The calculated results of the flow in the nozzle with mean expansion rate in divergent nozzle part $\dot{\bar{P}} = 4500\ s^{-1}$ are described ($\dot{\bar{P}} = -(1/P)\cdot(dP/dt)$). The effects of heterogeneous and/or spontaneous nucleation and condensation are discussed and compared with experiment.

2. Steam Condensation in a Nozzle

A nucleation of two types exists in the water steam flowing in a nozzle or in a turbine: homogeneous (spontaneous) and heterogeneous. The homogeneous nucleation occurs during the expansion 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 nucleation occurs already on the chemical impurities contained in the superheated water steam.

Superheated water steam, expanding in nozzles or 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.

The solid particles insoluble in water and in the water steam form the first category. Concentration of the 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 are partly dissolved in the superheated steam and they are 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 [3]- e.g.: NaCl, Na_2SO_4, 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.

Figure 1 shows the expansion of the water steam, containing chemical impurities (first of all NaCl), in the phase transition zone of the convergent-divergent nozzle during transonic velocity flow.

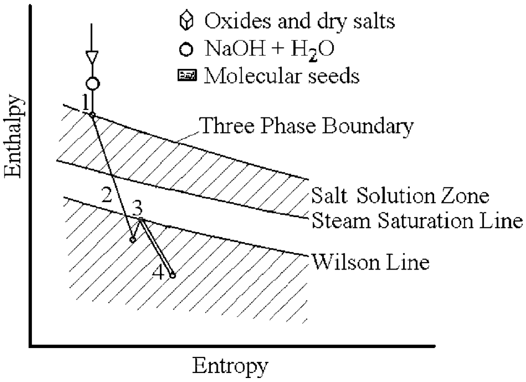

Fig. 1. Steam expansion line in phase transition zone.

The expansion in phase 1 first reaches the solution saturation line of the NaCl in the water, called three-phase boundary. This is at the top limit of the Salt Solution Zone (SSZ). The heterogeneous nucleation of the water molecules around the clusters of molecules or on molecules of NaCl, starts at this line.

The expansion goes through the SSZ in phase 2. The process of heterogeneous condensation continues even under the steam saturation line. The concentration of the heterogeneous droplets is usually not high enough for the condensation under the steam saturation line to occur in a thermodynamic equilibrium. A gradual subcooling of the steam occurs which can end in a shock of spontaneous nucleation in phase 3 at the Wilson line. The spontaneous creation of the nucleation seeds occurs. A condensation occurs on these nucleation seeds and on heterogeneous droplets under the Wilson line in phase 4 until the wet steam reaches the final state at the nozzle outlet.

3. Computational Model and Code

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

The mathematical model of the spontaneous nucleation is based on the Becker-Doering relationship [4] for the nucleation rate that gives very good results for pure water steam. The Becker-Doering theoretical formula is corrected by empirical parameters - the condensation coefficient $\alpha_K = 1.00$ and Gibbs free energy 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 Lankas [5].

The two-population model of homogeneous and heterogeneous condensation requires equations that enable to follow two independent populations of droplets. The total wetness is here composed of two parts $y = y_{Het} + y_{Hom}$ that are given by homogeneous and heterogeneous condensation. There is also used equation, which describes mean radius changes of heterogeneous droplets [1].

The system is linked with equations describing growth of homogeneous and/or heterogeneous droplets by condensation in the zone under steam saturation line, starting from critical radius of droplets. The relation of Gyarmathy [6] is used for droplets of both types [1].

It is assumed that the model will be used only for small total wetness ($y < 0.05\text{-}0.06$ 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 computational model is supplemented by empirical equation for the NaCl solubility in superheated steam as a function of the temperature, density and pressure - see Harvey and Bellows [7]. The model is also supplemented by empirical equation for the saturation salt-concentration in the water of heterogeneous droplets created on NaCl clusters as a function of the pressure and boiling temperature – see Chia-Tsun Liu, Lindsay, Jr. [8].

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 spontaneous 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.Nucleation and Condensation in SSZ Nucleation of the steam on clusters of NaCl molecules, and on NaCl molecules in SSZ, is still an open problem. The concentration of the nucleation seeds in superheated steam depends first of all on the mass concentration of NaCl and of the other chemicals present in the superheated steam.

The experimental facility of CTU was supplied with steam from two oil-fired boilers with a steam capacity of 1.94 $kg.s^{-1}$ each, P_{max} = 8.0 bar, T = 180 °C. Water chemistry was controlled with trisodium phosphate (Na_3PO_4) and sodium hydroxide (NaOH) additions in the range of 10-20 ppm P_2O_5 (blowdown water) and pH = 8.5-9.5 (feedwater), according to the Czech standard procedure CSN 07 7401 [2].

The purity of water steam was: Na < 25 ppb, Cl < 25 ppb, $S0_4$ < 15 ppb, PO_4 < 10 ppb, dissolved organics DO < 30 ppb. The low steam purity influenced no doubt the condensation process. The concentration of nucleation seeds could be high enough to produce extensive heterogeneous nucleation in SSZ. For instance the mass concentration of 1 ppb NaCl is equal to the molecule concentration of $1.03 \cdot 10^{16}$ kg^{-1}.

The saturation concentration of NaCl in water $W_{2max} \cong 28$ % at the three-phase boundary corresponds to the nucleation embryo composed of 1 molecule of NaCl and 8 molecules of H_2O. Due to the very low solubility of NaCl in water steam at low densities (about 0.1–0.3 ppt) - see [7], we can await mainly presence of NaCl clusters in the superheated steam and also in the nucleation embryos. The radius of nucleation embryos at the three-phase boundary for $W_{2max} \cong 28$ % in dependence on the rate of NaCl molecules in the cluster shows the tab.1.

Table 1. Radius of heterogeneous nucleation embryo.

Rate of NaCl molecules	1	10	100	1000
Embryo radius [nm]	0.41	0.88	1.90	4.08

As the droplets grow on the nucleation embryos in SSZ, the concentration of NaCl decreases in them and latent heat is simultaneously created. That pushes the passage of the expansion line through the steam saturation line to the lower pressure value. At the steam saturation line, the concentration of NaCl in the droplets should be so low that from the thermodynamic point of view they should be pure water droplets. This population of water droplets, created by heterogeneous nucleation, is taken into a consideration in our computational model.

In the computational model, it is assumed as an internal boundary condition, that heterogeneous water droplets of a mean radius and of a concentration are generated along the steam saturation line.

Experiments showed that the mean radius of droplets at the outlet of investigated nozzle and also in turbine stages, after the whole condensation process, is in the region around 100 nm [2, 9].

We can assume that the mean radius of heterogeneous droplets at the steam saturation line is in the range 5 - 50 nm. The calculation results show very small influence of this mean radius value on the condensation process in contrast to the value of heterogeneous droplets concentration in steam.

4. Computational Model Application

Two-population numerical model was applied for the calculation of the flow with condensation in nozzle with expansion rate in divergent nozzle part $\dot{P} = 4\ 500\ s^{-1}$. The same nozzle was used in experiments performed at CTU [2].

4.1. 2D Nozzle and Flow Mode The shape of the nozzle is obvious from the enclosed figures. The throat of nozzle is 0.048 m.

The parameters of the flowing steam are taken from the experiments. The total inlet parameters are: P_{at} = 2.5 bar, T_{at} = 418.15 K. It follows from the steam parameters shown that the inlet total temperature $\underline{T}_{at}$ corresponds to a superheating $(T_{at} - T_s)$ = 17.6 K. The flow in the nozzle is transonic and steam condensation occurs.

For the droplets at the steam saturation line, created by the heterogeneous nucleation in the SSZ, the values of droplet radius were tested: R_{Het} = 5.0 nm, 10 nm, 50 nm. The concentration of heterogeneous droplets was found by fitting of calculated pressure distribution in the nozzle to experimental one.

4.2. Calculation Results and Discussion Figure 2 shows the distribution of NaCl solubility $\underline{S}$ in superheated water steam in the nozzle.

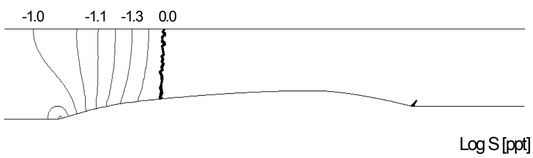

Fig. 2. Solubility (Log S [ppt]) of NaCl in superheated water steam in the nozzle.

The values of NaCl solubility in superheated steam, based on data of Harvey and Bellows [7], are very low with the maximum value S ≅ 0.2 ppt. It follows that NaCl is upstream of the nozzle inlet first of all in form of clusters of molecules.

The zone of the heterogeneous nucleation can be seen in Fig. 3. The contours of the equilibrium top concentration of NaCl in the droplets during the heterogeneous nucleation in SSZ are noticeable.

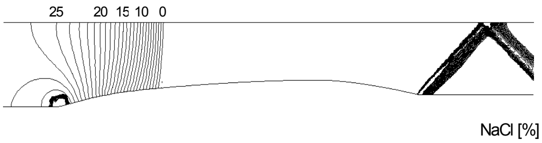

Fig. 3. Saturation concentration of NaCl [%] in SSZ droplets in the nozzle.

SSZ is located in the front part of the nozzle passage. It starts at the three-phase boundary and ends at the steam saturation line. We can not see the three-phase boundary in Fig. 3 because the steam parameters at the nozzle inlet correspond the attendance of SSZ.

The calculated courses of relative pressure P/P_{th}, with referential pressure at the nozzle throat $\underline{P}_{th}$, along the divergent part of the nozzle straight wall are visible from Fig. 4. The mean value of heterogeneous droplet radius at the steam saturation line was estimated R_{Het} = 1.0 e-8 m. It is possible to observe the position and shape of spontaneous condensation shock in dependence on the heterogeneous droplets concentration N_{Het}. The course of relative pressure shows a jump at the end of spontaneous nucleation zone.

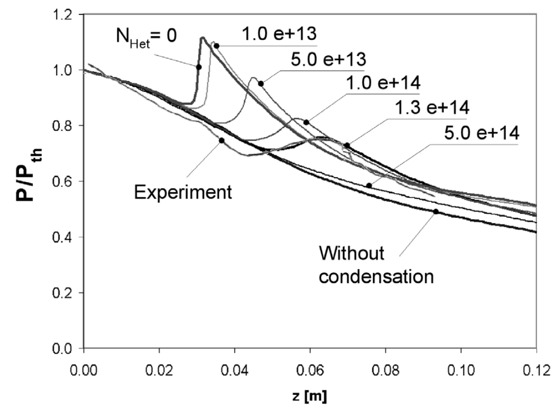

Fig. 4. Relative pressure P/P_{th} along the straight wall of divergent nozzle part, R_{Het} = 1.0 e-8 m.

The concentration of heterogeneous droplets found by fitting of calculated pressure distribution in the nozzle to experimental one has the value N_{Het} = 1.3 e+14 kg^{-1}. This concentration is low when taking in account very high mass concentration of NaCl in the steam. That is why we can await the presence of NaCl clusters in the superheated steam and also in the nucleation embryos.

Figure 5. illustrates very small effect of the heterogeneous droplet radius in the interval R_{Het} = 5.0 e-9 - 1.0 e-8 m on the pressure distribution and a negligible difference for bigger heterogeneous droplets.

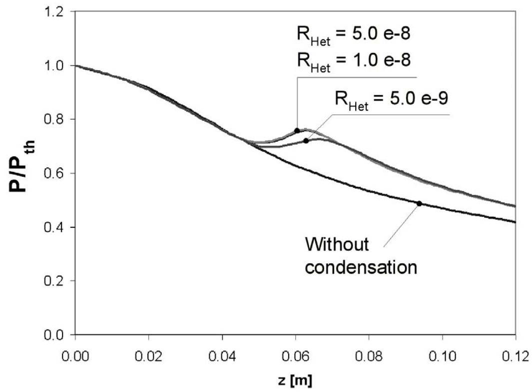

Fig. 5. Relative pressure P/P_{th} along the straight wall of divergent nozzle part, N_{Het} = 1.3 e+14 kg^{-1}.

Further figures illustrate the calculation results of the flow regime with heterogeneous droplets originated in SSZ of concentration N_{Het} = 1.3 e+14 kg^{-1} and mean radius R_{Het} = 1.0 e-8 m.

The zone of the spontaneous nucleation is noticeable in Fig. 6 showing the distribution of the spontaneous nucleation rate in the form of Log J contours.

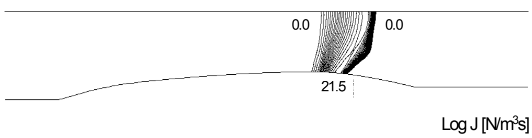

Fig.6. Spontaneous nucleation rate (Log J[$Nm^{-3}s^{-1}$]) in the nozzle.

The onset of the spontaneous nucleation is located at the nozzle throat. Figure 7 shows the courses of some nucleation and condensation parameters along the straight wall of the nozzle.

The zone of heterogeneous nucleation in SSZ is visualised by the course of NaCl concentration W2 in the droplets.

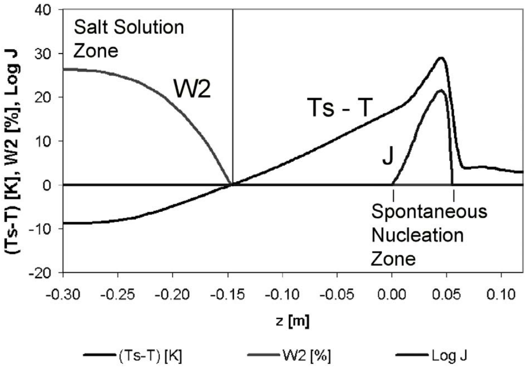

Fig. 7. Concentration of NaCl in droplets of SSZ W2, spontaneous nucleation rate J, subcooling (Ts - T) along the nozzle straight wall.

The zone of spontaneous nucleation is visualised by the course of nucleation rate in form of Log J. Downstream of the point of saturation, a fast subcooling (Ts - T) of the steam occurs with maximum value of $(Ts - T)_{max} = 28$ K. In the rear part of the nozzle subcooling decreases in direction to the outlet reaching the value of 3 K.

The steam wetness increases from the value of the heterogeneous wetness at the point of saturated steam; see Fig. 8. In front of the nozzle outlet reaches the value of $y_{Het} = 0.011$ kg.kg^{-1}.

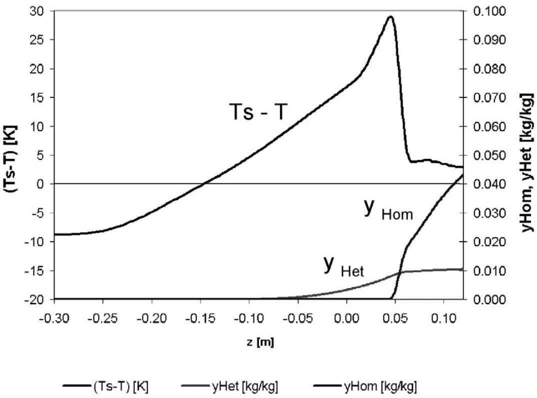

Fig. 8. Subcooling (Ts-T), heterogeneous wetness y_{Het}, homogeneous wetness y_{Hom} along nozzle straight wall.

The wetness contained in the droplets created by the spontaneous nucleation reaches in front of the nozzle outlet the value of $y_{Hom} = 0.043$ kg.kg^{-1}.

Figure 9 shows the calculated courses of the homogenous and heterogeneous droplets' radii. Their sizes increase in the direction of nozzle outlet.

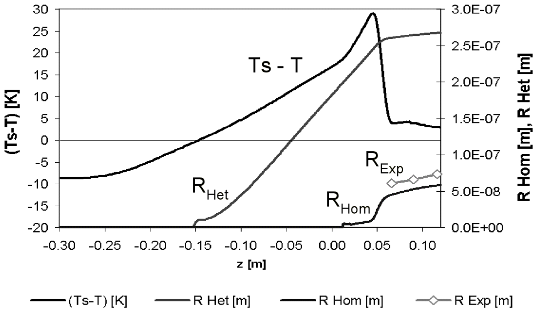

Fig. 9. Subcooling (Ts-T), heterogeneous droplet radius R_{Het}, homogeneous droplet radius R_{Hom}, experiment R_{Exp} along the nozzle straight wall.

In front of the nozzle outlet, the droplets originated by the heterogeneous nucleation reach mean size of $R_{Het} = 2.7$ e-7 m. It is noteworthy that the small heterogeneous droplets grow quickly in the region close behind the saturation line. The droplets created by the spontaneous nucleation reach the size of $R_{Hom} = 6.0$ e-8 m with the concentration of $N_{Hom} = 4.8$ e+16 kg^{-1}. They grow very quickly at the end of spontaneous nucleation.

Figure 9 shows also experimental data of Petr and Kolovratnik [2]. Droplet sizes were measured by light attenuation beginning from the nozzle throat (attenuation in the throat was supposed zero). The sizes of measured droplet radii are similar to the calculated sizes for homogeneous droplets. This matter of fact could be explained by much higher total mass and concentration of homogeneous droplets against heterogeneous ones.

5. Conclusions

The numerical simulations of the flow in a nozzle and comparison of computational results with experiment show some main pieces of knowledge.

The values of NaCl solubility in superheated steam upstream of the nozzle are very low with the maximum value S ≅ 0.2 ppt. It follows that NaCl is in superheated steam first of all in form of molecule clusters.

The zone of the heterogeneous nucleation in SSZ can be seen by means of the contours of NaCl saturation concentration in the nucleation embryos and in the droplets. The steam parameters at the nozzle inlet correspond the attendance of SSZ.

A very small effect of the size of heterogeneous droplets originated in SSZ on the nozzle flow was observed.

The concentration of heterogeneous droplets found by fitting of calculated pressure distribution in the nozzle to experimental one has the value N_{Het} = 1.3 e+14 kg^{-1}. This concentration is low in comparison with very high mass concentration of NaCl and other chemicals in the steam. We can await first of all presence of NaCl clusters in the superheated steam and also in the nucleation embryos.

The onset of parallel spontaneous nucleation is located at the nozzle throat. The zone of the spontaneous nucleation is noticeable by means of the contours of the spontaneous nucleation rate.

The course of relative pressure shows a jump at the end of homogeneous nucleation zone.

Downstream of the point of saturation, a fast subcooling of the steam occurs with maximum value 28 K. In the rear part of the nozzle subcooling decreases in direction to the outlet reaching the value of 3 K.

The wetness contained in the droplets originated by the spontaneous nucleation reaches in front of the nozzle outlet the value of y_{Hom} = 0.043 $kg.kg^{-1}$, whereas the heterogeneous wetness is only y_{Het} = 0.011 $kg.kg^{-1}$.

In front of the nozzle outlet, the droplets originated by the heterogeneous nucleation reach the size of R_{Het} = 2.7 e-07 m, whereas the homogeneous droplets reach the size of R_{Hom} = 6.0 e-08 m with the concentration N_{Hom} = 4.8 e+16 kg^{-1}.

The sizes of measured droplet radii are similar to the calculated sizes for homogeneous droplets. This matter of fact could be explained by much higher total mass and concentration of homogeneous droplets.

Good agreement of calculated results with experiment confirms the correctness of the developed computational model.

Weak points of experiment are absence of droplet measurements in SSZ and absence of measurements of chemical impurity concentrations in the steam during each experiment.

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