Assessment of condensation models for moist air transonic flow prediction

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Abstract. The aim of this article is to thoroughly analyse the influence of condensation models on the modelling of condensation phenomena in transonic flow of moist air. The reason for the study was the fact that different condensation models are used by researchers to obtain satisfactory results of numerical modelling. The condensation models tested herein differ in the nucleation rate formula and the droplets growth equation. Four most often used condensation models were selected for detailed investigations. The results obtained from each model were compared with experiments for the nozzle flow. The main focus was on the location of the onset of the nucleation process. Moreover, the droplets growth intensity was compared and discussed. The nozzle flow CFD calculations were performed using the ANSYS Fluent commercial tool. Finally, the condensation model which is the most suitable for the moist air transonic flow was recommended.

1 Introduction

The presence of water or steam in atmospheric air exerts a significant influence on flow conditions in elements of any devices or machines, affecting their durability, accuracy and efficiency. If unfiltered or wet, atmospheric air always contains a certain amount of suspended solid particles, water droplets (fog, rain, etc.) or steam. Air cleaning or drying is not feasible in many technical applications, e.g. in turbine engines. Therefore the impact of such impurities on the flow in turbomachinery needs to be investigated.

In the case of transonic flows, based on the condensation trigger, phase change phenomena can be divided into homogeneous and heterogeneous processes. Spontaneous nucleation occurs due to the process of rapid supersaturation (or supercooling) of gas, when the appearing condensation nuclei reach the critical radius triggering the homogeneous condensation phenomenon. If air contains suspended particles, condensation may occur on them. This process is referred to as heterogeneous condensation. The tiny droplets formed due to nucleation or on the suspended particles grow further. In favourable conditions they can reach significant sizes and form so-called coarse droplets. The condensation process can

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be rapid, especially during gas expansion in the convergent-divergent nozzle (CD nozzle), where supersonic conditions are reached in the nozzle divergent part. The phase change phenomena are connected with the interphase latent heat exchange. During the condensation process, latent heat is released from condensing steam to the gaseous phase. This affects the flow structure by changing the gas pressure, temperature and, thereby, velocity. The influence of the latent heat release is of major importance during the occurrence of rapid homogeneous condensation. The so-called condensation wave then appears, followed by a sudden release of a high amount of energy. On the other hand, if air contains suspended particles, heterogeneous condensation becomes the major phase-change process, which has a more gradual character but results in the formation of droplets with a relatively large size, depending on the initial size of the foreign nuclei.

Evaporation is a process contrary to condensation. If the droplet evaporates, latent heat is absorbed from the gaseous phase in the phase-change process, leading to a local drop in the fluid temperature, pressure, and therefore – in its density, velocity, entropy, etc. If the flow is supersonic, shock waves form, and the liquid droplets interacting with the shock wave tend to evaporate. This process is particularly interesting if the liquid fraction (e.g. fog or rain) is significant because it then results in the absorption of a relatively large amount of latent heat.

Most often homogeneous and heterogeneous condensation processes appear together. Only their share in the liquid phase formation may change depending on the air parameters. The parameter usually used to define the content of steam in humid air is called relative humidity, which is the relative value of the ratio of the mass of steam in the air to the total mass of steam the air can hold. Typical humidity values range from 40% to 50%. However, due to a change in weather conditions, the relative humidity level can reach as much as 100%. If the mass of steam in atmospheric air exceeds the mass of steam the air can hold, the excess of steam condenses creating fog. It has to be emphasized that the mass of steam that the air can hold, and therefore the air relative humidity, is strictly related to the air temperature and pressure. If the air temperature rises, the steam saturation pressure increases and, as a result, air can hold more steam. Therefore, the impact of temperature is crucial if condensation occurs. Another air parameter that has a major impact on phase-change phenomena is the number and diameter of the particles suspended in air. If the number of particles is significant, heterogeneous condensation might become the major phase-change phenomenon, weakening the influence of homogeneous condensation and weakening the condensation wave. Taking account of the impact of phase-change phenomena on the most crucial parameters of the transonic moist air flow, it must be stressed that the aforementioned factors (i.e., humidity, air parameters, presence of suspended solid or liquid particles) should be taken into consideration in CFD modelling of such flows.

Internal and external flows with condensation have been investigated intensively for over 50 years and are still of great interest to researchers all over the world [1]. In the 1960’s Gyarmathy proposed one of the most popular models for the droplet growth to model the steam condensing flow in the turbine. Gyarmathy’s model [2]was further modified by Young [3,4] and by Fuchs and Sutigin [5]in the 1970’s and provides slightly better predictions of the growth of nanosized droplets. The experimental and numerical studies regarding internal flows thorough CD nozzles conducted by Schnerr et al. [6,7,8] became the reference for researchers for the modelling of both moist air and pure steam condensing flows. Adam investigated, both experimentally and numerically, the non-stationarity of the flow, especially the impact of relative humidity on the interaction between condensation and shock waves and the oscillation frequency in a nozzle with parallel walls downstream the throat [10]. A 3D academic in-house code was developed by Dykas et al [9]. It treats the air-stream mixture as a homogeneous fluid and was validated against in-house experimental studies. The code enables robust computation of condensation in internal and external flows [12,13]. Recently, it became the basis for the model external implementation into commercial software. The functionality of the model implemented in the commercial software was extended by allowing slip velocity consideration, i.e. investigation of the difference between liquid and gaseous phase velocities, which is especially important if droplets reach a relatively large size or if the flow has a significant swirl [14,15]. Valuable techniques for condensation simulation in complex 3D structures were introduced by Yamamoto [16,17]. The numerical study of condensation is extremely demanding in terms of computing power, but the latest advancements have led to attempts to simulate the entire compressor rotor with a non-uniform circumferential distribution of wetness at the inlet [16]. The liquid water content at the jet engine inlet was studied by Moriguchi et al., who prove a significant change in air parameters at the compressor rotor outlet due to water evaporation [18]. Most numerical studies regarding condensation are performed based on the single-fluid approach, using the assumption of a continuous fluid for the mixture of air, steam and water. This approach gives reliable results if the droplet inertia and temperature between the phases are negligible. However, if the swirl of the flow of droplets is significant or if the droplets are relatively large, air and water should be considered as separate phases using the two-fluid approach. Some attempts have been made to model multi-phase humid air and wet steam flows [19,20,21]. Condensation is not only present in humid air. In fact, it is a very common phenomenon. Therefore, similar models have been adjusted to simulate condensation in pure steam [22,23,24,25,26,27] or in other gases, such as CO2 [28].

In this paper, the CFD computations are performed using the ANSYS Fluent commercial tool. The tool was extended by a condensation model using User Defined Functions (UDF's) [29]. The authors consider the influence of different condensation models on the condensation phenomena in the convergent-divergent nozzle.

2 Numerical and mathematical models

In this paper, the condensing flow is modelled numerically using the single-fluid approach, whereby the flow governing equations are stated for the mixture of air, steam and water. The slip velocity between the phases is neglected. All fluid properties, e.g. viscosity, thermal conductivity etc., are computed for mixture.

The RANS model for the compressible flow and the transport equations:

$$\frac{\partial}{\partial t}\rho+\frac{\partial}{\partial x_j}\rho\mathbf{v}_j=0 \tag{1}$$

$$\frac{\partial}{\partial t}\rho\mathbf{v}_i+\frac{\partial}{\partial x_{ij}}\left(\rho\mathbf{v}_i\mathbf{v}_{ij}+\delta_{ij}p-\boldsymbol{\tau}_{ij}\right)=0 \tag{2}$$

$$\frac{\partial}{\partial t}\rho E+\frac{\partial}{\partial x_j}\left(\mathbf{v}_j\rho E+\mathbf{v}_j p\right)=\frac{\partial}{\partial x_j}\left(k_{\text{eff}}\frac{\partial}{\partial x_j}T+\boldsymbol{\tau}_{ij}\mathbf{v}_j\right)+S_E \tag{3}$$

where ρ is density, t is time, **v** is the velocity vector, δ is Kronocker delta, p is pressure, **τ** is stress tensor, E is energy, k_{eff} is effective conductivity, T is temperature and S_E is source term due to condensation and it has following form:

$$S_E=\left(S_{y_{hom}}+S_{y_{het}}\right)\cdot L \tag{4}$$

where L is the latent heat.

The k-ω Shear-Stress-Transport (SST) model was adopted as the Eddy-Viscosity Turbulence Model [30]. The thorough description of the turbulence model can be found in ANSYS Fluent Theory Guide [31].

Additional transport equations were required to model the phase change duto homogeneous and heterogeneous condensation. Partial differential equations (PDEs) were included that describes the number of droplets per kilogram (*n*), created due to the nucleation process, and the liquid mass fraction (*y*), due to the homogeneous and heterogeneous condensation. These additional transport equations were introduced using the ANSYS Fluent UDFs. In total, there are three additional PDs, which in case of 2D flow, together with the RANS model, gives a system of 9 PDEs to solve. The number of solid particles in the heterogeneous process is constant and based on the literature and our previous research [32,14,9]. The additional transport equations for the liquid phase take the following form:

$$\frac{\partial \rho y_{hom}}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \mathbf{v}_j y_{hom}\right) = S_{y_{hom}} \tag{5}$$

$$\frac{\partial \rho n_{hom}}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \mathbf{v}_j n_{hom}\right) = S_{n_{hom}} \tag{6}$$

$$\frac{\partial \rho y_{het}}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \mathbf{v}_j y_{het}\right) = S_{y_{het}} \tag{7}$$

where S represents the source term: for eq. 5 – the source of mass of the condensed liquid due to homogenous condensation, for eq. 6 – the source of droplets per kilogram of air generated due to the nucleation process, for eq. 7 – the source of mass of water resulting from the heterogeneous condensation process. The source terms are defined by the following formulae:

$$S_{y_{hom}} = \frac{4}{3}\pi\rho\rho_l r^{*3} J_{hom} + 4\pi\rho\rho_l n_{hom} r_{hom}^2 \frac{\mathrm{d}r_{hom}}{\mathrm{d}t} \tag{8}$$

$$S_{n_{hom}} = \rho J_{hom} \tag{9}$$

$$S_{y_{het}} = 4\pi\rho\rho_l n_{het} r_{het}^2 \frac{\mathrm{d}r_{het}}{\mathrm{d}t} \tag{10}$$

where J is the nucleation rate presenting the number of nuclei with critical radius r^* formed in one kilogram of moist air in one second; r is the droplet radius, which is calculated based on the water mass fraction and number of droplets.

The homogeneous condensation process is triggered by spontaneous nucleation, whereby nuclei form in the fluid as the result of rapid supercooling, reaching the critical radius. In our model, the critical radius was based on the Kelvin equation:

$$r^* = \frac{2\sigma}{\rho_l R_v T_v \ln(S)} \tag{11}$$

where σ is the steam surface tension, R_v is the individual gas constant, T_v is the steam temperature and $S = p_v/p_s$ is supersaturation, the ratio of partial steam pressure to saturation pressure. The classical nucleation theory was implemented to describe the formation of condensation nuclei in one kilogram of moist air within one second. The nucleation rate corrected by Kantrowitz [33] is defined as:

$$J_{hom} = C\sqrt{\frac{2\sigma}{\pi m_v^3}}\frac{\rho_v}{\rho_l}\mathrm{e}^{\left(-\frac{4\pi r^{*2}\sigma}{3kT_v}\right)} \tag{12}$$

$$C = \frac{q_c}{1 + \frac{2(\gamma-1)}{(\gamma+1)}\frac{(h_v - h_l)}{R_v T_v}\left(\frac{(h_v - h_l)}{R_v T_v} - \frac{1}{2}\right)} \tag{13}$$

where γ is the ratio of specific heat capacities, m_v is the mass of one molecule, ρ_l is the liquid density at temperature T_v, k is the Boltzmann constant and q_c represents the condensation coefficient, which is equal to one.

The so-called non-isothermal Kantrowitz correction C is based on the assumption that all growing droplets have the same excess temperature. In the presence of a large volume of the gaseous phase, like in the case of moist air, the isothermal assumption is justified because collisions of condensing molecules with inert gas molecules are much more common than those with condensing droplets. Finally, it reduces nucleation by a factor of 50–100.

According to the gas dynamics theory, the frequency of the collision of steam molecules with condensation nuclei is related to the average free path of the steam molecules and the radius of the water droplets. The larger the Knudsen number (*Kn*), the smaller the diameter of the droplet. The equation for calculating *Kn* is:

$$Kn = \frac{l_S}{2r} = \frac{\mu_l\frac{\sqrt{9/8\pi RT}}{p}}{2r} \tag{14}$$

where ls is the free mean path of the steam molecule, μ is the dynamic viscosity of moist air, T is temperature, R is the gas constant; p is the pressure of moist air, r is the droplet radius.

When $Kn < 0.01$, the droplet growth process can be described as a continuous flow region. When $Kn > 4.5$, the droplet growth is governed by the free molecular flow. When $0.01 \leq Kn \leq 4.5$, the transition region is the case.

The most popular and the one most often used by researchers is the continuous droplet growth model developed by Gyarmathy [2], which is applied for a bigger size of droplets:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{1}{\rho_l}\cdot\frac{\left(1-\frac{r^*}{r}\right)}{r(1+3.18Kn)}\cdot\left(\frac{\lambda_v R_v {T_v}^2}{(h_v - h_l)^2}\right)\cdot\ln(S) \tag{15}$$

where λ_v is thermal conductivity of vapour.

The correction for this model was proposed in [3] and it is known as the Fuchs-Sutugin model:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{1}{\rho_l}\cdot\frac{(1+2Kn)\left(1-\frac{r^*}{r}\right)}{r(1+3.42Kn+5.32Kn^2)}\cdot\left(\frac{\lambda_v R_v {T_v}^2}{(h_v - h_l)^2}\right)\cdot\ln(S) \tag{16}$$

Another modification of Gyarmathy's model was proposed by Young, who, drawing on the experience from the nozzle flow modelling, introduced the following correction [3,4]:

$$\frac{\mathrm{d}r}{\mathrm{d}t}=\frac{1}{\rho_l}\cdot\frac{1}{r\left(1+3.78(1-v)\frac{Kn}{Pr}\right)}\left(1-\frac{r^*}{r}\right)\cdot\left(\frac{\lambda_v R_v {T_v}^2}{(h_v-h_l)^2}\right)\cdot\ln(S) \tag{17}$$

where:

$$v=\frac{R_v T_v}{(h_v-h_l)}\left(\alpha-0.5-\frac{2-q_c}{2q_c}\cdot\left(\frac{\gamma+1}{2\gamma}\right)\left(\frac{c_p T}{(h_v-h_l)}\right)\right) \tag{18}$$

coefficients α and q_c were set to 1 in the calculations presented herein.

In the continuous droplet growth models, the temperature of the droplets (T_l) can be determined by the capillarity effect using the expression given by Gyarmathy [2]:The correction for this model was proposed in [3] and it is known as the Fuchs-Sutugin model:

$$T_l=T_s-(T_s-T_v)\frac{r^*}{r}v \tag{19}$$

where T_s is the steam saturation temperature for given pressure. Here, steam temperature equals the temperature of air.

If the water droplets are very small, for which *Kn*>4.5, the growth of the droplets should be governed by considering the molecular and macroscopic transport process. The droplet growth equation for the free-molecular regime is given by the kinetic Hertz-Knudsen model [6,7,8]:

$$\frac{\mathrm{d}r}{\mathrm{d}t}=\frac{\alpha_c}{\rho_l}\cdot\frac{p_v-p_s}{\sqrt{2\pi R_v T}} \tag{20}$$

In eq.20 α_c is a condensation coefficient describing how many steam molecules colliding with the water droplet settle on its surface. The value of 1 for this coefficient means that all steam molecules are captured by the water droplet surface. If this value equals 0, none of the steam molecules are captured by the water droplet surface, all are deflected. For the Hertz-Knudsen droplet growth model, the droplets, steam and air have the same temperature: $T_v = T_l = T$.

3 Numerical study

The geometry of the circular nozzle presented below (Fig. 1) was applied to investigate moist air condensing flows using different droplet growth models. This nozzle was previously used in our numerical as well as experimental research [13,15]. The 2D mesh presented on Figure 1 was created and it has ~21 000 elements, the boundary layer with growth rate equal to 1.2 was introduced to obtain $y^+ = 1$. As a convergence criterion of the iteration process, it was assumed that the mass flow rate difference between inlet and outlet was less than 0.01%.

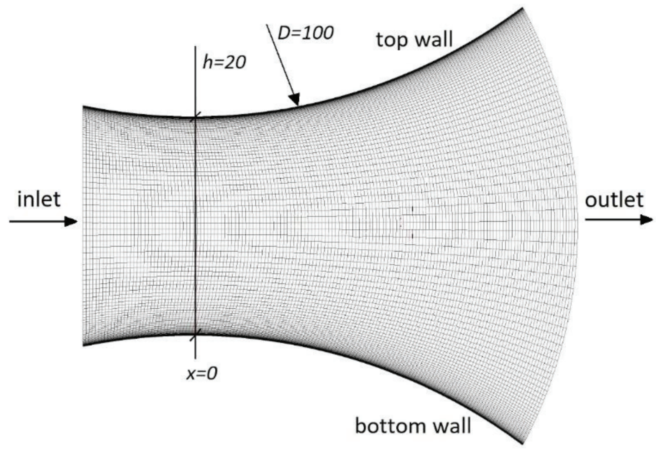

Fig. 1. Mesh of the applied circular nozzle

Bearing in mind that the homogeneous condensation process consists of nucleation and droplet growth phenomena, four different droplet growth models will be used below keeping the same nucleation model. The computational results will be compared with the experimentally obtained static pressure distribution along the central axis of the nozzle. The static pressure distribution reveals the location and intensity of the condensation process. The aim is to check which droplet growth model captures the experimental results in the best way.

Table 1 gathers the boundary conditions for the two cases corresponding to the experimental measuring campaigns [13] .

Table 1. Boundary conditions

	Case 1	**Case 2**
Relative humidity, %	43	68
Inlet total pressure, kPa	98.8	98.8
Inlet total temperature, K	297.15	297.15
Outlet	Supersonic	Supersonic

Generally, two types of the droplet growth model are considered: continuous and kinetic. The Knudsen number decides which model should be used (cf. eq. 14). Therefore, the steam molecule free mean path l_s should be determined first to find the size of the droplets that should be expected choosing one of the two types of the droplet growth model under consideration (Fig.2).

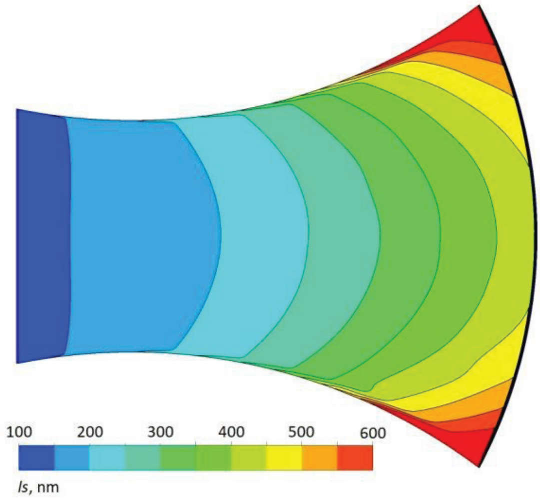

Fig. 2. Distribution of the free mean path of steam molecules

Analysing the values of the free mean path of the steam molecule (Fig. 2), it can be noticed that for the continuous droplet growth model the expected size of the droplet is bigger than $1 \cdot 10^{-5}$ m, which is much bigger than the size of droplets which are usually formed due to the nucleation process. In the case of moist air condensing flows, the so-called coarse droplets arise only when heterogeneous condensation takes place on the water droplets or solid particles already existing in the flow.

3.1 Comparison of droplet growth models

Due to the fact that in transonic condensing flows the range of the Knudsen number values can be wide, the use of the kinetic Hetrz-Knudsen (HK) droplet growth model seems to be a simplification. However, the majority of continuous droplet growth models already include a correction with respect to the Knudsen number, such as the Gyarmathy (GY), the Fuchs-Sutugin (FS), or the Young (YO) correction. Nevertheless, these corrections are rarely used in moist air condensing flow modelling. Fig. 3 presents a comparison of the moist air condensing flow modelling in a circular nozzle by means of four different droplet growth models. The simulation results were compared with the experimentally obtained static pressure distribution along the nozzle midline. The calculations results obtained from simulations using the Hertz-Knudsen (HK) model, with condensation coefficient α_c=1, and the continuous model with the Fuchs-Sutugin (FS) correction are similar and close to the experimental data. On the other hand, the continuous models with the Gyarmaty (FS) and the Young (YO) correction differ from the experiment significantly for both cases. For Case 1, with the lower relative humidity value, the HK and the FS droplet growth models are very close to each other, even in terms of the droplet size.

Using the continuous droplet growth model, information is obtained about the temperature difference between the droplet and steam $\Delta T = T_{\mathrm{l}} - T_{\mathrm{v}}$. In the case of the kinetic model it is assumed that this difference is zero. Fig. 4 presents the distribution of the rise in the droplet temperature due to condensation. The highest value of this temperature difference is observed for the model with the Fuchs-Sutugin correction.

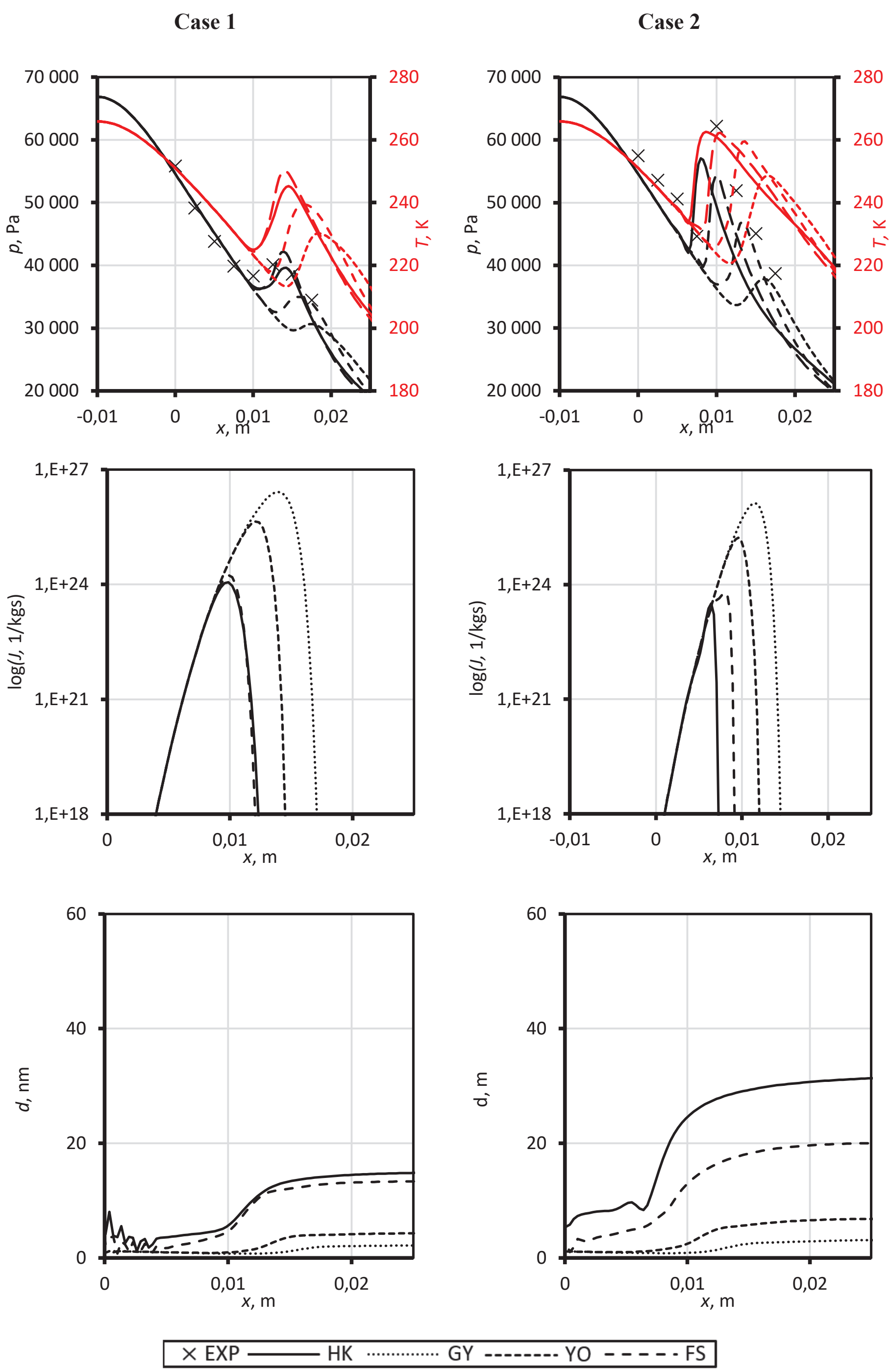

Fig. 3. Comparison of numerical results with different droplet growth models: static pressure and static temperature; nucleation rate and droplets size distributions along the nozzle axis

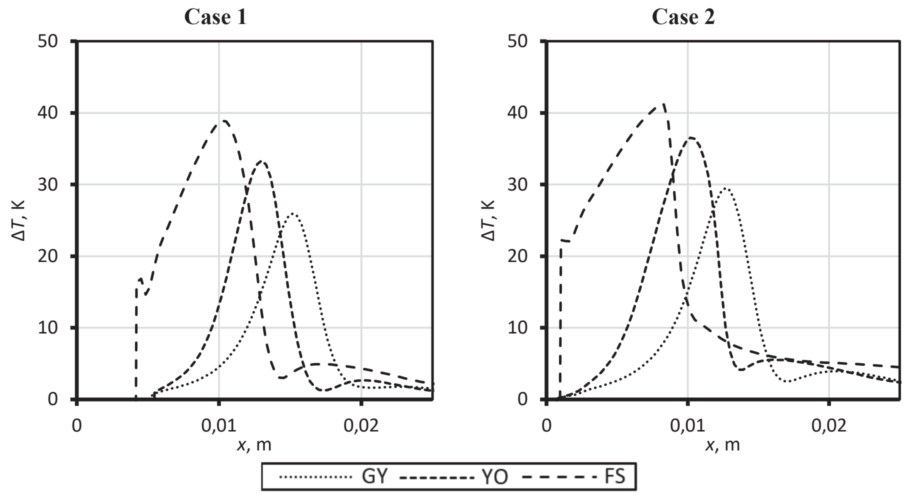

Fig. 4. Comparison of temperature difference $\Delta T = T_l - T_v$; distributions along the nozzle midline calculated using different continuous droplet growth models

4 Conclusions

The present numerical study investigates the suitability of different droplet growth models for the moist air condensing flow. The obtained results lead to the following conclusions:

- For moist air condensing flows where only homogeneous condensation is considered, the Hertz-Knudsen droplet growth model is recommended.
- The Fuchs-Sutugin correction for the continuous droplet growth model gives results close to the experiment, providing additional information on the temperature difference between the droplet and steam.
- Due to the wide range of the Knudsen number values, a hybrid droplet growth model is recommended, especially when heterogeneous condensation is considered as well.

Summing up, the paper shows that each selection of the condensation model should not be arbitrary and it requires a validation process first, for the experimental data for moist air flow, not steam flow. The study presented herein should make clear that the choice of droplet growth model depends on the flow conditions, what seems to be trivial, but in the case of heterogeneous condensation, it may be crucial.

Our future research in this field will concentrate on the application of the hybrid droplet growth model for the condensing flow modelling in more complex geometries.

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