



UNIVERSITÀ  
DEGLI STUDI  
FIRENZE

## FLORE

# Repository istituzionale dell'Università degli Studi di Firenze

### **CFD modeling of condensing steam ejectors: Comparison with an experimental test-case**

Questa è la Versione finale referata (Post print/Accepted manuscript) della seguente pubblicazione:

*Original Citation:*

CFD modeling of condensing steam ejectors: Comparison with an experimental test-case / Mazzelli, Federico\*; Giacomelli, Francesco; Milazzo, Adriano. - In: INTERNATIONAL JOURNAL OF THERMAL SCIENCES. - ISSN 1290-0729. - ELETTRONICO. - 127:(2018), pp. 7-18. [10.1016/j.ijthermalsci.2018.01.012]

*Availability:*

This version is available at: 2158/1122145 since: 2021-03-30T09:10:04Z

*Published version:*

DOI: 10.1016/j.ijthermalsci.2018.01.012

*Terms of use:*

Open Access

La pubblicazione è resa disponibile sotto le norme e i termini della licenza di deposito, secondo quanto stabilito dalla Policy per l'accesso aperto dell'Università degli Studi di Firenze (<https://www.sba.unifi.it/upload/policy-oa-2016-1.pdf>)

*Publisher copyright claim:*

Conformità alle politiche dell'editore / Compliance to publisher's policies

Questa versione della pubblicazione è conforme a quanto richiesto dalle politiche dell'editore in materia di copyright.

This version of the publication conforms to the publisher's copyright policies.

(Article begins on next page)

# CFD modeling of condensing steam ejectors: comparison with an experimental test-case

Federico Mazzelli\*, Francesco Giacomelli, Adriano Milazzo

Department of Industrial Engineering, University of Florence,  
via di Santa Marta, 3 – 50139 FIRENZE (ITALY)

## Abstract

In the present paper, a numerical model for the simulation of wet-steam flows has been developed and implemented within a commercial CFD code (ANSYS Fluent) via user defined functions. The scheme is based on a single-fluid approach and solves the transport equations for a homogeneous mixture coupled with conservation equations for the droplets number and liquid volume fraction. The model is validated against a steam nozzle test-case and then compared with experimental data from a steam ejector with a significant amount of generated liquid phase. The simulations show a good agreement both in terms of mass flow rates and pressure profile data. Some of the modeling assumptions are also reviewed and discussed.

**Keywords:** Wet-Steam; CFD; Experimental Test-Case; Steam Ejector; Non-Equilibrium Condensation

## Nomenclature

<i>Latin letters</i>		<i>Greek letters</i>	
$a$	Speed of sound [ $\text{m s}^{-1}$ ]	$\alpha$	Volume fraction [-]
$B$	Second virial coefficient [ $\text{m}^3 \text{kg}^{-1}$ ]	$\beta$	Mass fraction [-]
$C$	Third virial coefficient [ $\text{m}^6 \text{kg}^{-2}$ ]	$\Gamma$	Liquid mass generation rate [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
$c$	Specific heat capacity [ $\text{J kg}^{-1} \text{K}^{-1}$ ]	$\gamma$	Specific heat ratio [-]
$G$	Gibbs Free-Energy [J]	$\eta$	Droplets per unit volume mixture [ $\text{m}^{-3}$ ]
$h_{lv}$	Latent heat [ $\text{J kg}^{-1}$ ]	$\lambda$	Thermal conductivity [ $\text{W m}^{-1} \text{K}^{-1}$ ]
$J$	Nucleation rate [ $\text{s}^{-1} \text{m}^{-3}$ ]	$\zeta$	Kantrowitz non isothermal correction
$k_b$	Boltzmann constant [ $\text{J K}^{-1}$ ]	$\rho$	Density [ $\text{kg m}^{-3}$ ]
$k$	Turbulent kinetic energy [ $\text{m}^2 \text{s}^{-2}$ ]	$\sigma$	Surface tension [ $\text{J m}^{-2}$ ]
$l$	Molecular mean free path [m]	$\tau$	Shear stress [Pa]
$m$	Mass [kg]	$\varphi_{ss}$	Supersaturation ratio [-]
$n$	Droplets per unit mass of mixture [ $\text{kg}^{-1}$ ]	$\omega$	Specific dissipation rate [ $\text{s}^{-1}$ ]

\* Corresponding author: federico.mazzelli@unifi.it – 0039 055 2758740

$p$	Pressure [Pa]	<i>Subscripts</i>	
$q_c$	Accommodation factor	$d$	Droplet
$R$	Specific gas constant [ $\text{J kg}^{-1} \text{K}^{-1}$ ]	$m$	Mixture, molecule
$r$	Radius [m]	$v$	Vapor
$t$	Time [s]		
$T$	Temperature [K]		
$u$	Velocity [ $\text{m s}^{-1}$ ]		

## 16 1. Introduction

17 Non-equilibrium condensation of steam occurs in many jet and turbomachinery devices, such as supersonic  
18 nozzles, ejectors and low pressure stages of steam turbines. Normal operation of these devices involves flow  
19 expansions that leads to thermodynamic states that are well within the saturation dome. Due to the very limited  
20 residence time, however, thermodynamic equilibrium is not maintained and the water vapor reaches high levels  
21 of supercooling. At a certain degree of steam expansion, the vapor state abruptly collapses and condensation  
22 takes place as a shock-like disturbance, called the “condensation shock” [1]. This sudden change in the state  
23 of aggregation leads to an instantaneous and localized heat release that increases the pressure and temperature  
24 and reduces the Mach number. Moreover, the condensation shock implies large temperature differences  
25 between the phases that cause irreversibilities. Downstream of the condensation shock, the flow contains a  
26 considerable number of small liquid droplets (of the order of  $10^{19}/\text{dm}^3$ , [2]) that can interact in non-trivial ways  
27 with the carrier phase.

28 To date, CFD simulations of wet-steam flows have proved to achieve a quite good agreement for the steam  
29 condensation within transonic nozzles [3], both in terms of pressure and droplet size trends. However, the same  
30 may not hold true in ejector applications where the interaction between droplets, shocks and shear layers may  
31 introduce many unpredictable effects. In this respect, most of the numerical studies on condensing steam  
32 ejectors have been accomplished through single-phase, ideal-gas simulations (e.g., [4]) and very few examples  
33 of CFD using wet steam models exist (see for instance, [5], [6]). This lack of detailed simulations of condensing  
34 steam ejectors provides motivations for this study.

35 In order to accurately validate numerical simulation on ejector applications, the comparison with experimental  
36 data should be made by considering both global and local parameters. Unfortunately, articles reporting these  
37 type of data appears to be very few. In particular, the study of Chunnanond and Aphornratana [7], and the  
38 subsequent work of Sriveerakul *et al.* [4], provide results for the entrainment ratios and pressure profiles along  
39 the ejector walls. However, no information on the separate primary and secondary mass flow rates is given,  
40 which makes difficult the assessment of numerical results. In this work, the validation of the developed model  
41 is made by comparing the simulation results against two different experimental test-cases, the converging-  
42 diverging nozzle from Moses and Stein [8] and the supersonic steam ejector studied by Al-Doori [9] and  
43 Ariaifar *et al* [5], who provide data for both mass flow rates and wall pressure profiles.

## 73 2. Numerical Model

74 In the past decades, several methods have been devised to simulate wet steam flows, with different levels of  
 75 complexities and accuracy. The simplest and perhaps most used is the so-called “single-fluid” approach. This  
 76 is basically a fully Eulerian scheme that assumes the liquid phase to be uniformly dispersed within the vapor  
 77 volume. The mass, momentum and energy conservation equations are written for the homogeneous two-phase  
 78 mixture and two further equations describes the conservation of the droplets number and liquid mass within  
 79 the computational domain. This method is commonly employed by commercial codes (e.g. ANSYS Fluent or  
 80 CFX) and has been used by several research teams [5] [6] [10].

81 A second method, called the “two-fluid” approach, is very similar to the previous one, with the exception that  
 82 the conservation equations are solved for the two phases separately. This can result in greater accuracy thanks  
 83 to the possibility of describing the energy and force exchange between the phases. On the other hand, modeling  
 84 the interphase interaction is a complex task that can potentially lead to larger uncertainties than with the use  
 85 of simpler models (especially in ejectors, where the wet-steam flows across shear layers and shocks). The two-  
 86 fluid method has been investigated by many authors, who have either adapted commercial codes [11] or  
 87 developed in-house solvers [12] [13].

88 To date, wet steam models are available in many commercial CFD codes that generally feature models based  
 89 on the single-fluid approach. Although these codes dispense from developing complex in-house solvers, the  
 90 use of built-in models does not allow freedom in the change of model parameters and settings. This work  
 91 represents an attempt to overcome this limitation through the development of a customized model within a  
 92 widely used CFD commercial code. This approach has the double benefit of allowing great flexibility in the  
 93 choice of the physical model and, at the same time, exploiting the capability of commercial software in terms  
 94 of solver settings.

95 The scheme developed in this work is based on the single-fluid approach. The conservation equations for mass,  
 96 momentum and energy are written for the average mixture fluid and assume the form of the conventional  
 97 Navier-Stokes equations for compressible flows:

98

$$\begin{aligned}
 \frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_{mj}}{\partial x_j} &= 0 \\
 \frac{\partial \rho_m u_{mi}}{\partial t} + \frac{\partial \rho_m u_{mi} u_{mj}}{\partial x_j} &= -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij\_eff}}{\partial x_j} \\
 \frac{\partial \rho_m E_m}{\partial t} + \frac{\partial \rho_m u_{mj} H_m}{\partial x_j} &= \frac{\partial q_{j\_eff}}{\partial x_j} + \frac{\partial u_{mi} \tau_{ij\_eff}}{\partial x_j}
 \end{aligned} \tag{1}$$

99

100

In eq. (1), the properties of the mixture are described by means of mass or volume weighted averages:

101

$$\begin{aligned}
 \varsigma_m &= \beta \varsigma_l + (1 - \beta) \varsigma_v \\
 \chi_m &= \alpha_l \chi_l + (1 - \alpha_l) \chi_v
 \end{aligned} \tag{2}$$

128

129 where  $\zeta_m$  represents mixture thermodynamic properties like enthalpy, entropy, total energy, etc...,  $\chi_m$  is the  
130 mixture density, molecular viscosity or thermal conductivity,  $\beta$  is the liquid mass fraction and  $\alpha_l$  is the liquid  
131 volume fraction. The connection between these last two quantities is straightforward:

132

$$\beta = \frac{m_l}{m_l + m_v} = \frac{\alpha_l \rho_l}{\alpha_l \rho_l + (1 - \alpha_l) \rho_v} \quad (3)$$

133

134 The evaluation of the mixture speed of sound requires special considerations [14], and is calculated here by  
135 means of an harmonic average:

136

$$a = \sqrt{\frac{1}{(\alpha_l \rho_l + \alpha_v \rho_v) \left( \frac{\alpha_l}{\rho_l a_l^2} + \frac{\alpha_v}{\rho_v a_v^2} \right)}} \quad (4)$$

137

138 Coupled with the transport equation for the mixture are the two equations for the conservation of the liquid  
139 mass and the droplets number:

140

$$\frac{\partial \rho_m n}{\partial t} + \frac{\partial \rho_m u_{mj} n}{\partial x_j} = \alpha_v J \quad (5)$$

$$\frac{\partial \rho_l \alpha_L}{\partial t} + \frac{\partial \rho_l u_{mj} \alpha_L}{\partial x_j} = \Gamma \quad (6)$$

141

142 where “ $n$ ” is the number of droplets per unit mass of the mixture and it is assumed that the two phases move  
143 at the same speed (no-slip condition).

144 The term “ $J$ ” in eq. (5) represents the nucleation rate, i.e., the rate of formation of new droplets per unit  
145 volume of vapor and is expressed here through the classical nucleation theory (more details can be found in  
146 [15]) modified with the Kantrowitz non-isothermal correction [16]:

147

$$J = \frac{q_c}{(1 + \xi)} \frac{\rho_v^2}{\rho_l} \left( \frac{2\sigma}{\pi m^3} \right)^{1/2} \exp\left(-\frac{\Delta G^*}{k_b T_v}\right) \quad (7)$$

$$\xi = q_c \frac{2(\gamma - 1)}{(\gamma + 1)} \frac{h_{lv}}{RT_v} \left( \frac{h_{lv}}{RT_v} - \frac{1}{2} \right)$$

148

149 Where  $q_c$  is the accommodation factor,  $h_{lv}$  is the liquid-vapor latent heat,  $\sigma$  is the liquid water surface tension  
150 and  $\xi$  is the Kantrowitz non-isothermal correction.

151 This correction is needed when the rapidity of the nucleation process prevents the two phase from reaching the  
152 thermal equilibrium (i.e.,  $T_L = T_v$ ). In the case of fast transformations (or low heat transfer rate between the

181 phases) the temperature in the cluster becomes greater than  $T_v$  due to the latent heat release. This localized heat  
 182 release enhances the rate at which the molecules evaporate from the cluster surface and leads to a partial  
 183 suppression of the critical nucleation rate  $J$ . The Kantrowitz' correction reproduces this phenomenon and  
 184 typically reduces  $J$  by a factor of 50–100 [15].

185 The term  $\Delta G^*$  in eq. (7) is Gibbs Free energy needed to form a stable liquid cluster (other thermodynamic  
 186 constants are defined in the nomenclature). Thermodynamic stability considerations lead to a simple  
 187 expression for  $\Delta G^*$  [17]:

188

$$\Delta G^* = \frac{4}{3}\pi r^{*2}\sigma \quad (8)$$

189

190 Where  $r^*$  is the critical radius of a stable liquid cluster:

191

$$r^* = \frac{2\sigma}{\rho_l R T_v \cdot \ln \varphi_{ss}} \quad (9)$$

$$\varphi_{ss} = \frac{P_v}{P_{sat}(T_v)}$$

192

193 where  $\varphi_{ss}$  is the supersaturation ratio.

194 Equations (7) - (9) give the rate at which liquid nuclei spontaneously form within the vapor stream. The  
 195 presence of the exponential term in eq. (7) is indicative of the shock-like nature of the condensation  
 196 phenomenon. Moreover, it is important to note that all the variables of equations (7) - (9) depend solely on  
 197 the vapor thermodynamic state.

198 In order to close the set of governing equations, it is necessary to provide a law for the liquid mass generation  
 199 rate per unit volume of mixture,  $\Gamma$ , in eq. (6). This quantity stems from two different sources:

200

$$\Gamma = \Gamma_{nuc} + \Gamma_{grow} = \alpha_v m_d^* J + \rho_m n \frac{dm_d}{dt} \quad (10)$$

201

202 where  $m_d$  is the mass of a generic liquid droplet and  $m_d^*$  is its value when the liquid nucleus first forms. By  
 203 assuming a spherical shape for all liquid droplets, these are given by:

204

$$m_d^* = \frac{4}{3}\pi \rho_l r^{*3}$$

$$m_d = \frac{4}{3}\pi \rho_l r_d^3 = \frac{\rho_l \alpha_l}{\rho_m n} \quad (11)$$

205

206 The first of the two terms in the RHS of eq. (10) describes the mass generated from freshly nucleated droplets.  
 207 This term is significant only in the first stages of the condensation process and is rapidly overtaken by the

249 second addendum,  $\Gamma_{grow}$ , which represents the growth or shrinkage of existing droplets. Its expression requires  
250 the definition of a droplet growth law. In this work we use the formulation derived by Hill following a statistical  
251 mechanics approach [2] and later rearranged by Young [18]:

$$\frac{dr_d}{dt} = \frac{p_v}{\rho_l h_{lv} \sqrt{2\pi RT_v}} \frac{c_p + c_v}{2} \cdot (T_s(p_v) - T_v) \quad (12)$$

253  
254 Equations from (1) to (12) form a closed system of equations that can be solved as long as the vapor and  
255 liquid equations of state and thermodynamic properties are provided. In this respect, calculations of the non-  
256 equilibrium phase-change of steam necessarily requires the description of the fluid properties in metastable  
257 conditions, meaning that common tabulated properties cannot be used to this purpose. Unfortunately, there is  
258 a serious lack of experimental data for the properties of steam in supercooled conditions, which is regularly  
259 testified by reports of the International Association for the Properties of Water and Steam (IAPWS) [19].  
260 Consequently, it is necessary to extrapolate a generic equation of state outside its normal range of validity in  
261 order to describe metastable states within the saturation curve.

262 In the present work, the steam properties are calculated following the work of Young [20] who derived a Virial  
263 equation of state truncated at the third term of the expansion:

$$p = \rho_v RT_v \cdot (1 + B\rho_v + C\rho_v^2) \quad (13)$$

265  
266 where  $B$  and  $C$  are the second and third Virial coefficients. These are function of the sole temperature and their  
267 expressions were calibrated to match steam data in the range between 273.16 and 1073 K. Moreover,  
268 formulations for the enthalpy, entropy and specific heats are derived from the Virial equations based on a  
269 procedure described by Young [20]. The steam thermal conductivity and dynamic viscosity are given by low  
270 order polynomial functions of the vapor temperature obtained from interpolation of NIST dataset [21]. The  
271 liquid phase properties (viz., liquid density, specific heat capacity, thermal conductivity and viscosity) are  
272 calculated assuming saturation conditions and are again expressed through empirical correlations obtained  
273 from NIST [21]. Finally, the water surface tension is a function of the sole temperature and is expressed  
274 following Young [18].

275 The described model has been implemented within the commercial CFD package ANSYS Fluent v18.0 [22].  
276 In this regard, ANSYS Fluent features a built-in Wet Steam model that exploits a specifically developed  
277 density based solver. Unfortunately, it is not possible to directly modify the nucleation rate and droplet growth  
278 laws of this model according to user defined schemes. Nevertheless, the set-up of a customized scheme is still  
279 possible within the framework of Fluent pressure-based multiphase solver by adding a number of User Defined  
280 Functions (UDF). Of these, three are needed to input the source terms for the liquid mass fraction and droplet  
281 number transport equation and to enforce the expression for the diameter of the droplets. Moreover, a User  
282 Defined Real Gas Model is required to implement the virial equation of state and transport properties of the

313 vapor phase. Ultimately, it may be worth to note that, although density-based solvers generally perform better,  
314 pressure-based schemes have also been successfully applied for the simulations of multiphase compressible  
315 flows with discontinuities (e.g. [23]). In the next section, the accuracy of the developed pressure-based scheme  
316 will be assessed by comparison with results from the Fluent density based model.

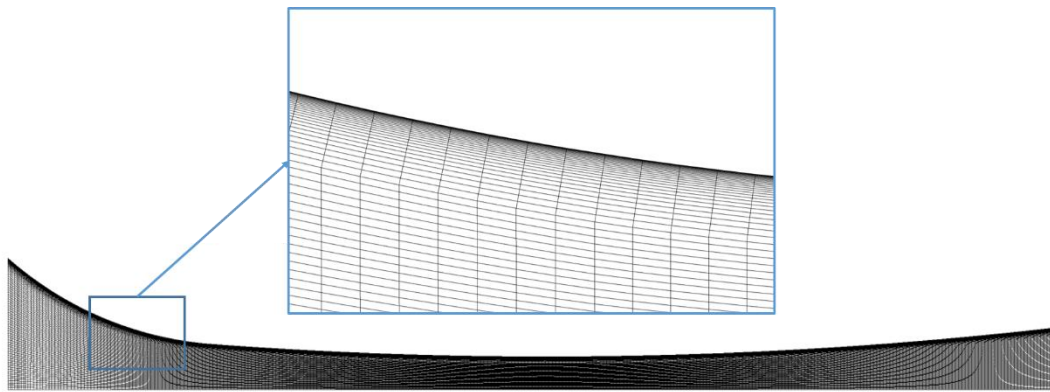
317

### 318 3. Steam Nozzle

319 In what follows, the presented numerical model is compared against data from the well-known nozzle test case  
320 of Moses and Stein [8]. The results are firstly also confronted with those obtained with the ANSYS Fluent  
321 built-in wet steam model in order to benchmark the present scheme with a previously validated code (e.g., [24]  
322 [25]). In this comparison, the droplet generation and growth rates equations implemented in the customized  
323 model are the same as those featured by the Fluent built-in scheme. Subsequently, we address the analysis of  
324 changes in some of the model's settings (e.g., the droplet growth law).

325 The computational domain for these simulations has approximately 30'000 quadrilateral cells with  $y^+ < 1$  along  
326 the nozzle surfaces and is presented in [Fig. 1](#). Due to the relative simplicity of the flow field (e.g., absence of  
327 pressure shocks), it was possible to set-up a third order accurate QUICK scheme [26] for the spatial  
328 discretization of all transport equations. A  $k-\omega$  SST turbulence model is selected for all simulations.

329



330

331 *Fig. 1 – Computational domain for the nozzle test-case*

332

333 Simulations are performed for the experiment n. 252, which has inlet total pressure of 40 kPa and inlet total  
334 temperature of 101.2 K [8]. For this test, data on pressure profiles and liquid mass fraction along the axis are  
335 available. Results on droplet average radius were not presented in the original paper; however, these were  
336 processed by Young [18] starting from light scattering data.

337 [Fig. 2](#) shows the normalized pressure trend along the ejector axis. The figure focuses on the region downstream  
338 of the nozzle throat (located at  $x=8,22$  cm from the nozzle inlet) where the condensation shock takes place and  
339 experimental measurements are available. Clearly, the presented model overlaps with results from the Fluent  
340 built-in model and both seem to capture the pressure trend with reasonable accuracy. When compared to



369 experimental values, numerical results underestimate the general pressure level and the steepness of the  
 370 pressure rise.

371 [Fig. 2](#), presents also the comparison on the average droplet radii along the nozzle axis. The results show that  
 372 CFD predicts values that are approximately a half of the experimental. Nevertheless, it is known that for this  
 373 particular test-case there is a general tendency to under-predict droplet sizes by CFD models [3].

374 It is interesting to note that the numerical trends for the average radius tend to predict different slope of the  
 375 curve in the region where the nucleation has terminated. This difference is even more pronounced when  
 376 comparing the trends for the number of droplets per unit volume of mixture, as shown in [Fig. 3](#). The figure  
 377 clearly shows two different trends of the numerical codes. In particular, the Fluent built-in model predicts the  
 378 presence of a plateau immediately downstream of the nucleation zone, whereas the developed model shows a  
 379 decreasing trend in this region.

380 The reason for this difference is to be found in the formulation for the droplet number conservation, eq. (5).  
 381 In the present study, the equation is written in term of the conservation of the droplets per unit mass of mixture,  
 382 which, once multiplied by the mixture density, returns the number of droplets per unit volume:

383

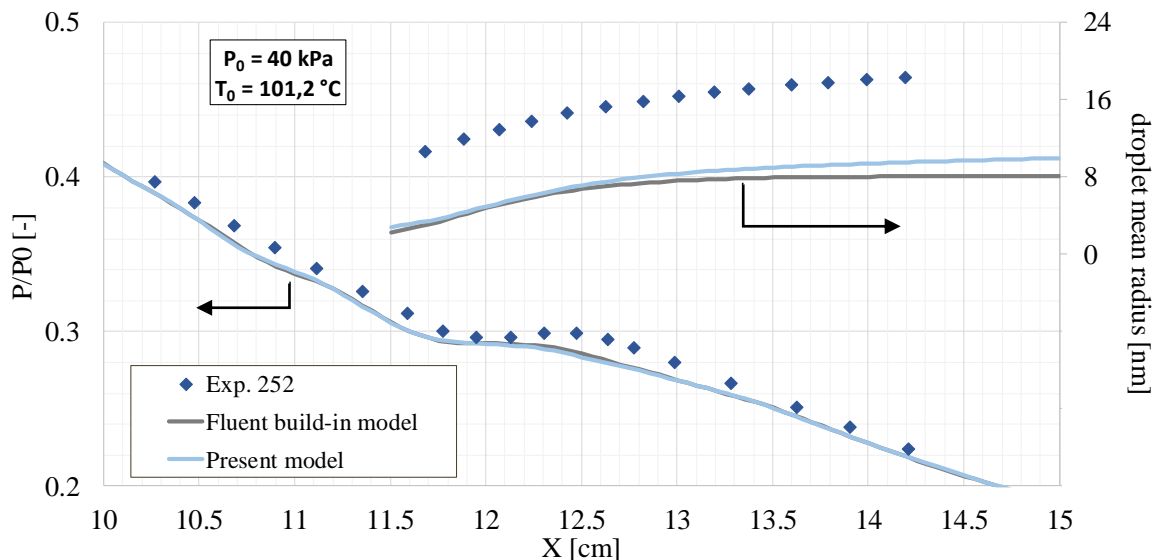
$$\eta = \rho_m n \quad (14)$$

384

385 where  $\eta$  is the number of droplets per unit volume of mixture (or number density).

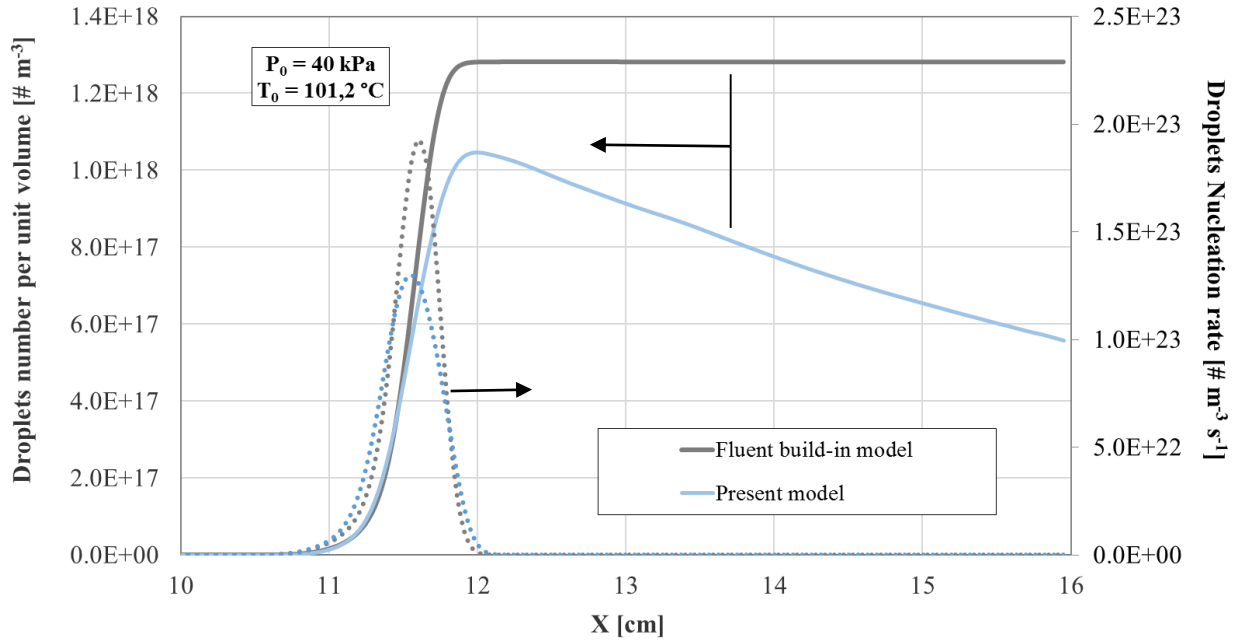
386 Writing eq. (5) in these terms allows the total number of droplets to be conserved in the computational domain,  
 387 which is simply shown by performing a volume integration of the LHS of eq. (5), (the conservation of the  
 388 droplet number can equally be obtained by using  $\eta$  as a variable, as long as the proper corrections to the droplet  
 389 nucleation term,  $J$ , are made). Consequently, the present model improves on the Fluent built-in scheme by  
 390 correctly reproducing a decreasing trend for  $\eta$ . This is caused by the fact that the total number of nuclei  $n$  is  
 391 constant in this region (the nucleation rate is zero) and the flow is expanding in a duct with increasingly larger  
 392 sections.

393



394

399 Fig. 2 – Normalized pressure trend along the nozzle axis (bottom curves) and corresponding droplet average  
 400 radius (top right curves)  
 401



402  
 403 Fig. 3 – Number of droplets per unit volume of mixture along the nozzle axis (solid lines) and the  
 404 corresponding droplets nucleation rates (dotted lines)  
 405

406 **Sensitivity to different model settings**

407 In this section, we present an analysis of the sensitivity to some of the most influential parameters of the phase  
 408 change model, i.e., the surface tension, the nucleation equation and the droplet growth law. Specifically, we  
 409 first evaluate the impact of suppressing the Kantrowitz non-isothermal correction from the nucleation equation.  
 410 Secondly, we describe the surface tension by using an empirical correlation from IAPWS [19]. Lastly, we  
 411 analyze the use of a widely used droplet growth law that was derived by Young [18] starting from an equation  
 412 obtained by Gyarmathy [27]. Its final expression is as follows [3]:

413

$$\frac{dr_d}{dt} = \frac{\lambda_v}{\rho_l h_{lv} r_d} \frac{\left(1 - \frac{r^*}{r_d}\right)}{\left(\frac{1}{1 + 2C_1 Kn} + 3.78(1 - v) \frac{Kn}{Pr}\right)} \cdot (T_s(p_v) - T_v) \quad (15)$$

$$v = \frac{RT_s}{h_{lv}} \left( C_2 - 0.5 - \frac{2 - q_c}{2q_c} \left( \frac{\gamma + 1}{2\gamma} \right) \left( \frac{c_p T_s}{h_{lv}} \right) \right) \quad (16)$$

414

415 where  $\lambda_v$  is the vapor phase thermal conductivity,  $Pr = \mu c_p / \lambda_v$  is the Prandtl number and  $Kn$  is the Knudsen  
 416 number, defined as the ratio between the droplet diameter and the molecular mean free path:

452

$$Kn = \frac{l}{2r_d} \quad (17)$$

453

454 The two constants  $C_1$  and  $C_2$  in eq. (15) and (16) represents two tunable modelling parameters (see [18] for  
455 a description of their significance) that are set respectively equal to 0.0 and 9.0, as suggested by Young [18].

456 [Fig. 4](#) shows the comparison of the different model settings for four experimental cases (Exp. 252, 257, 193  
457 and 411; for these last two measurements of the diameters are not available). Clearly, the use of the non-  
458 isothermal correction significantly retards the nucleation process with respect to the isothermal case. In turn,  
459 this results in a better agreement with experiments in all the simulated cases.

460 The adoption of the IAPWS correlation for the surface tension does not result in any detectable difference with  
461 respect to the formulation proposed by Young [18]. This is because the difference in the surface tension as  
462 predicted by the two correlations is always lower than 0.1% (at least for the range of temperature of interest  
463 for this study). However, it is important to note that both these formulation describes the surface tension as a  
464 function of the sole temperature and disregard any potential influence of the curvature radius.

465 Although it is generally acknowledged that the surface tension depends on the curvature for very small droplet  
466 radii (especially below 10nm [28], which is the range of interest for wet steam flows), experimental evidences  
467 are still required to specify how  $\sigma$  depends on  $r$  or even identify the sign of this variation (some studies suggest  
468 that this may be temperature-dependent, with a transition from positive to negative upon increasing T above  
469  $\sim 250$  K [28]). Moreover, due to its chief impact on the nucleation process ( $\sigma$  appears within the exponential  
470 term of eq. raised to the third power) any change in the expression for the surface tension most likely requires  
471 a complete recalibration of the physical model settings and constants. As a result, most of the previous works  
472 in the wet steam related literature have been accomplished exploiting the simplified flat-film surface tension  
473 assumption, as in this study.

474 Finally, the most interesting comparison in [Fig. 4](#) relates to influence of the droplet growth law. The analysis  
475 of the various results reveals that the Young's droplet growth law can better capture the experimental trends  
476 for the average radius. By contrast, the two laws appear to alternatively match the experimental trends for the  
477 pressure, with the Young's law that always anticipate the nucleation region with respect to the Hill's  
478 expression.

479 This fact can be explained by considering the specific calibration adopted for the Young's droplet growth law.  
480 In particular, it is known that higher values of  $C_2$  (as in this case) serve to boost the growth rate, resulting in  
481 larger droplets whilst simultaneously shifting the pressure rise upstream [3]. The analysis of other boundary  
482 conditions not reported here confirms the alternating performance of the two models. Therefore, it is not  
483 possible at present to draw a definite conclusion as to which model performs the best and both these expressions  
484 are tested for the analysis of the steam ejector.

485 Finally, it should be mentioned that the uncertainty connected to the pressure measurements was estimated by  
486 Moses and Stein [8] to be about  $\pm 40$  Pa (the corresponding error bars are approximately of the same size of

Elimi

Elimi

Elimi

Form

Form

Elimi

491 the experimental symbols in Fig. 4). In terms of droplet radius, Starzmann et al [3] make reference to an  
 492 estimated uncertainty of perhaps  $\pm 20\%$ , although the details of the derivation are not reported.

493

494

495

496

497

498

499

500

501

502

503

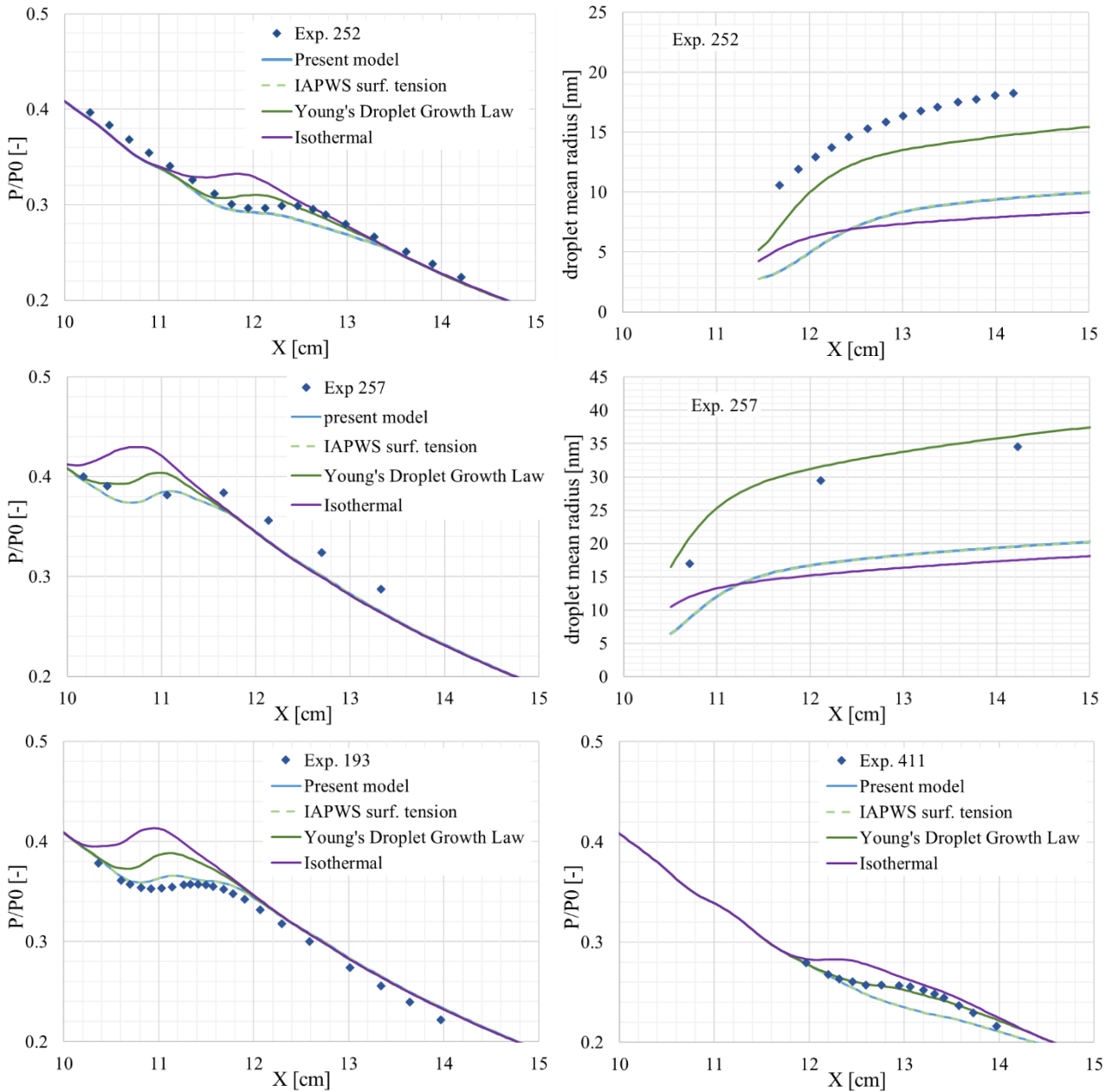


Fig. 4 – Comparison of model settings for different cases: Exp. 252 ( $P_0=40050$  Pa,  $T_0=374.3$  K), Exp. 257 ( $P_0=67661$  Pa,  $T_0=376.7$  K), Exp. 193 ( $P_0=43023$  Pa,  $T_0=366$  K), Exp. 411 ( $P_0=42276$  Pa,  $T_0=385.15$  K)

## 4. Steam Ejector

In this section, the developed model is validated against data from the supersonic steam ejector studied by Al-Doori [9] and Ariaifar *et al* [5].

534 The set of boundary conditions analyzed are summarized in [Table 1](#). The solution of the governing equations  
 535 is achieved exploiting a pressure-based coupled solver. A second order accurate up-wind scheme is selected  
 536 for the spatial discretization of all transport equations except for the volume fraction and momentum equations.  
 537 The first of these is discretized through a 3<sup>rd</sup> order QUICK scheme whereas for the latter a power-law scheme  
 538 had to be chosen due to numerical instabilities connected with the pressure-velocity coupling.  
 539 A k- $\omega$  SST turbulence model is selected for all the simulations because of the specific calibration for transonic  
 540 applications [29] and based on previous studies on single phase ejector flows [30] [31]. In addition, due to the  
 541 high Mach reached within the ejector mixing chamber, two additional UDFs are built to endow the turbulence  
 542

543 *Table 1: Summary of ejector boundary conditions*

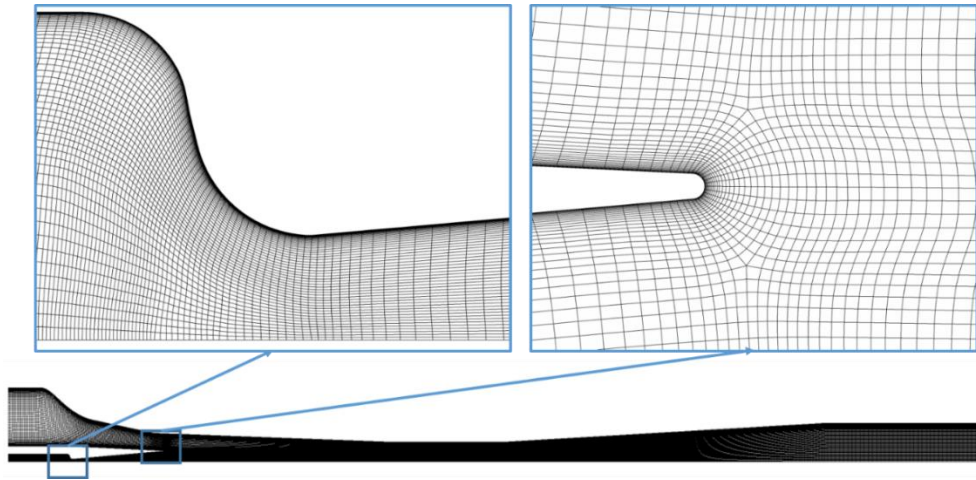
Stream	Total Temperature [K]	Total Pressure [kPa]
Motive	403	270
Suction	287	1.6
Discharge	From 4.2 to 7.5 static pressure	

544  
 545 model equations with the correction for compressible mixing layer (in ANSYS Fluent, these are available only  
 546 for single-phase flows).

547 [Fig. 5](#), shows the computational domain used for all the CFD analyses. Due to the high directionality of the  
 548 flow (axial velocity component always greater than transversal component), a structured grid is selected to  
 549 reduce numerical diffusion. Moreover, a straight channel is added at the end of the domain, due to the presence  
 550 of large recirculation regions at the ejector outlet that prevented reaching stable convergence for some  
 551 operating conditions. Although this change may induce some approximations, these are most probably limited  
 552 to a small region near the outlet (the flow upstream of the shock in the diffuser is not influenced due to the  
 553 hyperbolic nature of the supersonic flow). Moreover, the inclusion of the channel prevents backflow of  
 554 unknown characteristics from entering into the ejector and allows the recirculation to reattach within the  
 555 computational domain, thus improving the numerical stability of the simulations.

556 The adequacy of the mesh refinement was checked by comparing the mass flow rates results for three different  
 557 grids having all  $y^+$  values less than 1 along the ejector surfaces. [Table 2](#), shows the results of the study. In order  
 558 to reduce the computational time, the grid with 70k quadrilateral cells is selected for all subsequent  
 559 calculations.

560 Convergence of the solution is defined by an error in the mass flow imbalance of less than  $10^{-5}$  kg s<sup>-1</sup> and  
 561 calculations are stopped when all residuals are stable. Walls are assumed to be adiabatic and smooth.  
 562  
 563



590

591 Fig. 5 – Computational domain and mesh details of the primary nozzle throat and fillet (grid with 70k cells)

592

593

Table 2: Grid independence study

Grid cells	Mass flow rate [kg/s]			Difference with finer mesh		
	Motive	Suction	ER	Motive	Suction	ER
~35 000	0.00341	0.00111	0.327	0.5%	-13.0%	-13.4%
~70 000	0.00339	0.00128	0.377	0.1%	1.2%	1.1%
~140 000	0.00338	0.00126	0.373	-	-	-

594

595

### Entrainment Ratio and mass flow rates

596

597 [Fig. 6](#) shows the comparison between the experimental and numerical Entrainment Ratio (ER) curves. Both the Young's and Hill's droplet growth law are tested (hereafter referred as Yg82 and Hi66). Details of the experimental apparatus and measurement procedures can be found in [9] (chapter 4 and 5). According to Al-Doori [9] the uncertainty level for the ER is around  $\pm 3\%$ . The numerical simulations produce a higher value of ER at on design with a percent difference of about 14%. Moreover, CFD models somewhat anticipate and smoothen the transition toward the off design regime.

602

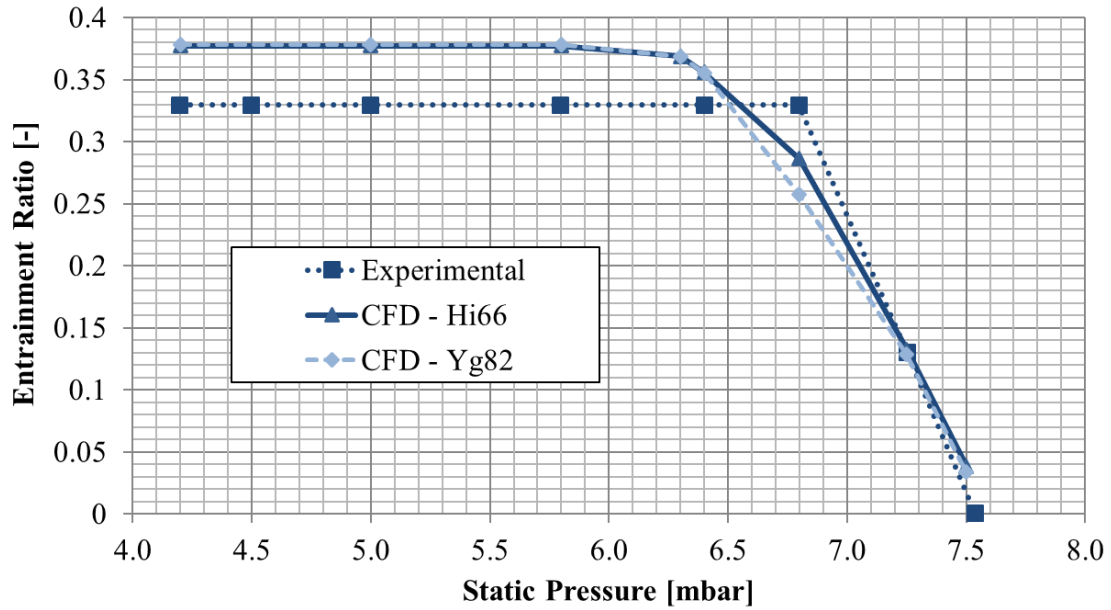
603 Despite the large discrepancy, [Fig. 7](#) illustrates that when results for the motive and suction flows are analyzed separately, differences are smaller than the corresponding value of ER. This is due to a summation of the errors when dividing the two quantities (in other studies, the authors have found that the discrepancy was lower for the ER than the mass flow rates, as in [30]). In particular, the greatest discrepancy is achieved for the data of the suction flow rates, with a percent difference of about 7% at on design, whereas the difference for the motive flow rate is slightly less than 6%. For these two quantities, Al-Doori [9] reports uncertainties of 0.6% and 1-2% for the primary and secondary mass flow rate, respectively.

609

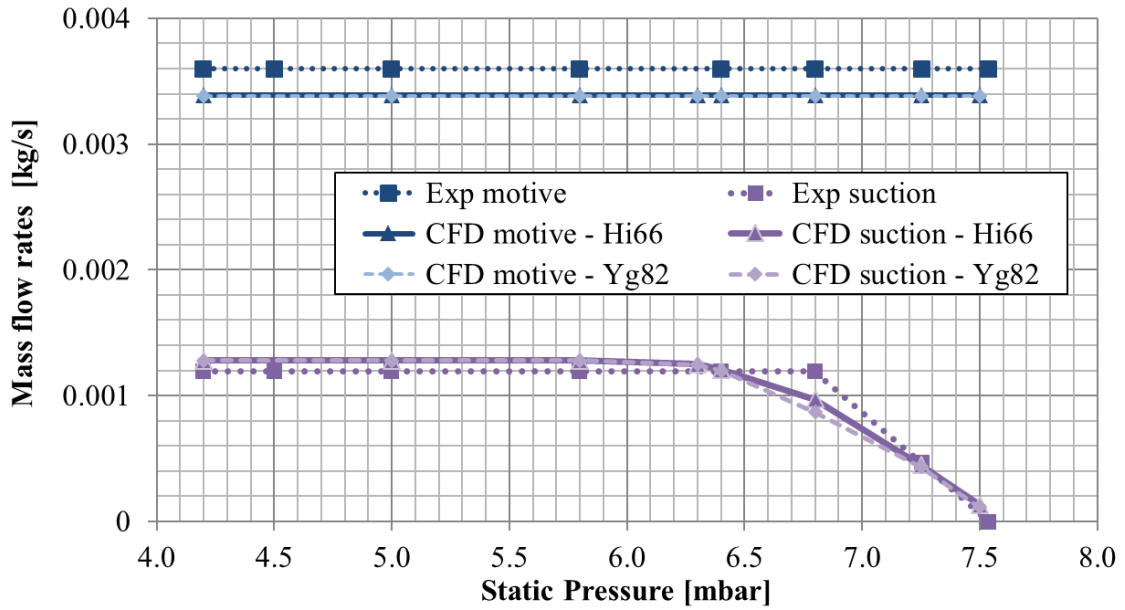
610 In terms of models sensitivity, the change of the droplet growth law seems to have a limited influence on the ejector mass flow rates. The only minor change occurs at off design, where the Hill's model performs slightly better than the Young's law. Moreover, a check of many flow variables has revealed only minor differences between the two models, as illustrated in [Fig. 8](#) for the volume fraction and Mach profile along the ejector

612

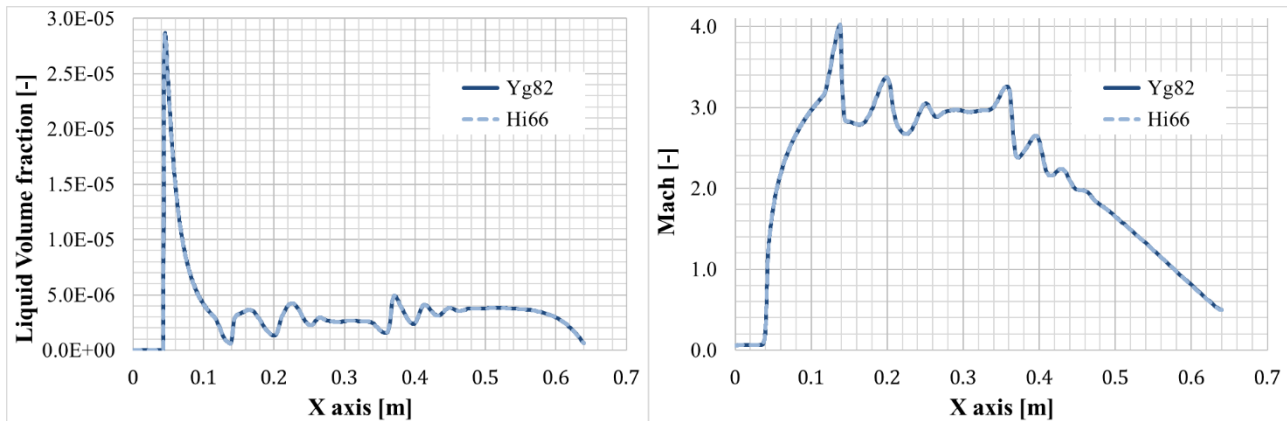
616 axis. Consequently, all the subsequent analyses in this paper are carried out by considering only the Hill's  
 617 droplet growth expression.  
 618



619  
 620 *Fig. 6 – Comparison of experimental and numerical ER (experimental data are taken from [9])*  
 621



622  
 623 *Fig. 7 – Comparison of experimental and numerical mass flow rates (experimental data are taken from [9])*  
 624



652

653

654

655

Fig. 8 – Liquid Volume Fraction (left) and Mach Number (right) profiles along the ejector axis. Comparison of different droplet growth models ( $P_{out} = 4.2 \text{ kPa}$ )

656

### Accuracy of mass flow rates predictions

657

658

659

660

661

662

663

Despite the general trend for ER being well reproduced, the discrepancy on the primary flow rate is still large compared with the error that should reasonably arise from the simulation of the 1D flow across a De Laval nozzle. A first possible cause for this discrepancy may come from numerical inaccuracies due to the low grid refinement and low order discretization (especially for the momentum equation). In order to check this hypothesis, a grid/order independence was performed solely on primary nozzle and the results are shown in [Table 3](#). Clearly, despite some differences between the low and high order schemes remaining even for the finest mesh, the scatter is in all cases well below the 1%.

664

665

666

667

668

669

670

671

672

673

674

675

One further reason for the discrepancy of the primary flow rate may be the presence of liquid at motive inlet (it should be noted that no superheating was imposed in the experimental tests). This may increase the average density of the stream passing through the throat, producing a larger value of experimental flow rate. Moreover, the presence of liquid nuclei or steam impurities (such as solid particles) may strongly affect the intensity and type of the condensation process (see for instance [12]). In this respect, a sensitivity analysis was performed by varying the amount of liquid mass fraction at nozzle inlet (the simulations were performed for the 22k nozzle mesh with the 3 order accurate scheme). The results of these trials showed that in order to increase the motive mass flow rate of about 6%, it is necessary to impose nearly 15% of liquid mass fraction at inlet<sup>1</sup>, which is a too large amount to explain the discrepancy with experiments. Nevertheless, these trials were performed with the single-fluid approach described previously. This method is generally not suited to investigate problems with secondary or multiple nucleation [32]; hence, the obtained results cannot exclude the presence of liquid nuclei at the motive inlet, which could have an impact on the experimental trends.

676

677

678

Finally, one further cause may be the uncertainty connected with the experimental measurements and with the geometrical dimension of the throat. As for the first, Al-Doori [9] estimates an uncertainty of around 0.6% for the primary mass flow rate, which is almost one order of magnitude lower than the differences with CFD. On

<sup>1</sup> This indicates that change in flow rate does not linearly depend on density variations, for instance, adding 6% percent of mass fraction at inlet leads to an increase of around 1.5% of the primary flow rate



680 the other hand, previous studies performed on a single phase air ejector [30] have shown that even small  
681 uncertainties in the throat dimension (connected mostly with the manufacturing process), can lead to  
682 discrepancies in the mass flow rate up to many percents. Unfortunately, Al-Doori does not report information  
683 on the geometrical uncertainty and manufacturing precision for the investigated profiles. Nevertheless, a first  
684 estimation of the sensitivity to the nozzle throat diameter can be achieved by making use of the compressible  
685 1D equations for perfect gases.

686 By considering an average specific heat ratio of 1.3 (as found from inspection of CFD results), this method  
687 returns a primary mass flow rate  $\sim 0.00336$  kg/s, which is around 1% lower than CFD results. By making use  
688 of this simple approach, it is found that an increase of only  $16 \mu\text{m}$  (i.e., 1% of the nominal diameter) produce  
689 a change of the mass flow rate of more than 2%. If we consider this estimated sensitivity to approximately  
690 hold for CFD simulations, it follows that a discrepancy of around  $50 \mu\text{m}$  may provide a difference close to the  
691 one obtained in the present simulations.

692 It is concluded that both the presence of liquid at inlet and possible geometrical uncertainties may have played  
693 a role in the observed differences with experimental primary flow rate.

694

695 *Table 3: Motive nozzle mass flow rates for different grid size and discretization schemes*

Discr. order Grid size	1 <sup>st</sup> order	Present setup	Full 2 <sup>nd</sup> order	3 <sup>rd</sup> order
$\sim 22\ 000^*$	3.388 E-03	3.388 E-03	3.369 E-03	3.371 E-03
$\sim 44\ 000$	3.376 E-03	3.378 E-03	3.363 E-03	3.365 E-03
$\sim 88\ 000$	3.376 E-03	3.376 E-03	3.357 E-03	3.357 E-03

696 \*this is the mesh size used for the ejector calculations

697

698 We focus now on the suction flow rate. From a general viewpoint, it is known that accurate predictions of the  
699 entrainment process requires accounting the influence of compressibility on the mixing layer. In particular,  
700 experimental investigations performed in the 70s (e.g., [33] [34]) have shown that compressible mixing layers  
701 are affected by a significant reduction of the spreading rate with respect to equivalent low-speed  
702 configurations.

703 Although this effect has been known for a long time, no convincing theoretical explanation has been given yet  
704 and turbulence models predict this decrease empirically (see Smits and Dussauge [35] or Gatsky and Bonnet  
705 [36] for more details). For  $\omega$ -based models, Wilcox [37] proposes a correction to the turbulence kinetic energy  
706 equation based on the turbulent Mach number:

707

$$Ma_t = \frac{\sqrt{2k}}{a} \quad (18)$$

708

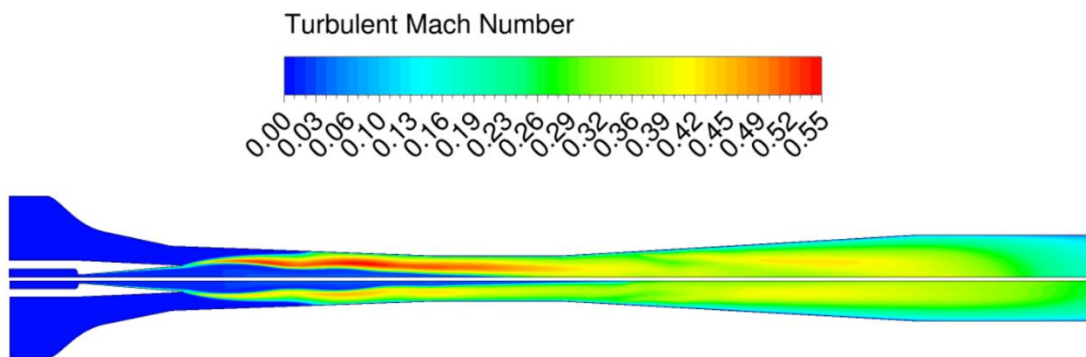
709 where  $k$  is the turbulent kinetic energy and  $a$  is the speed of sound.

710 The compressibility correction reduces the mixing layer entrainment by increasing the dissipation of  
711 turbulence kinetic energy within shear layers. Although its use improves the accuracy for compressible mixing

741 layers, the correction can negatively affect predictions for wall boundary layers at transonic and supersonic  
742 speeds [38]. Because of this, the application of the correction was carefully evaluated.

743 [Fig. 9](#) shows a comparison of the turbulent Mach number field between a simulation with the compressibility  
744 correction active and one without correction. As can be seen, the turbulent Mach reaches very high levels  
745 within the mixing layer and downstream of the shock in the diffuser. In particular, a substantial part of the  
746 mixing layer presents values of  $Ma_t$  larger than 0.25, which is the threshold for compressibility to have any  
747 impact on the mixing layer [38]. The use of the correction limits these peak values and reduces the mixing  
748 layer spreading rate. In turn, the suppression of the spreading rate results in a reduction of the suction flow rate  
749 of nearly 17% percent. Therefore, the difference with the experimental mass flow rate would be of about 22%  
750 without the compressibility correction (as opposed to the 7% obtained with the correction).

751



752

753 *Fig. 9 – Turbulent Mach number contour for the case with compressibility correction (bottom) and without*  
754 *compressibility correction (top) ( $P_{out} = 4.2 \text{ kPa}$ )*

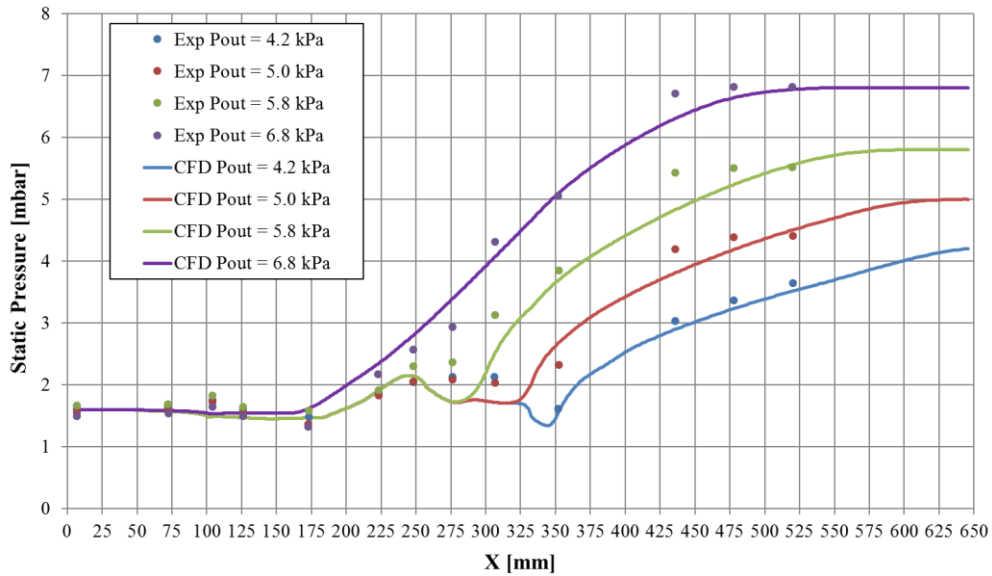
755

### 756 **Wall Pressure Profile**

757 [Fig. 10](#) presents the results for the pressure profiles along the ejector wall. In order to perform the comparison,  
758 the outlet boundary conditions were imposed so as to match the value of the last pressure probe in the diffuser.  
759 This was necessary due to the presence of large recirculations along the diffuser that prevented the pressure  
760 recovery from completing at the ejector outlet (it should be noted that the straight channel attached downstream  
761 of the diffuser begins at  $x = 535.5 \text{ mm}$ ).

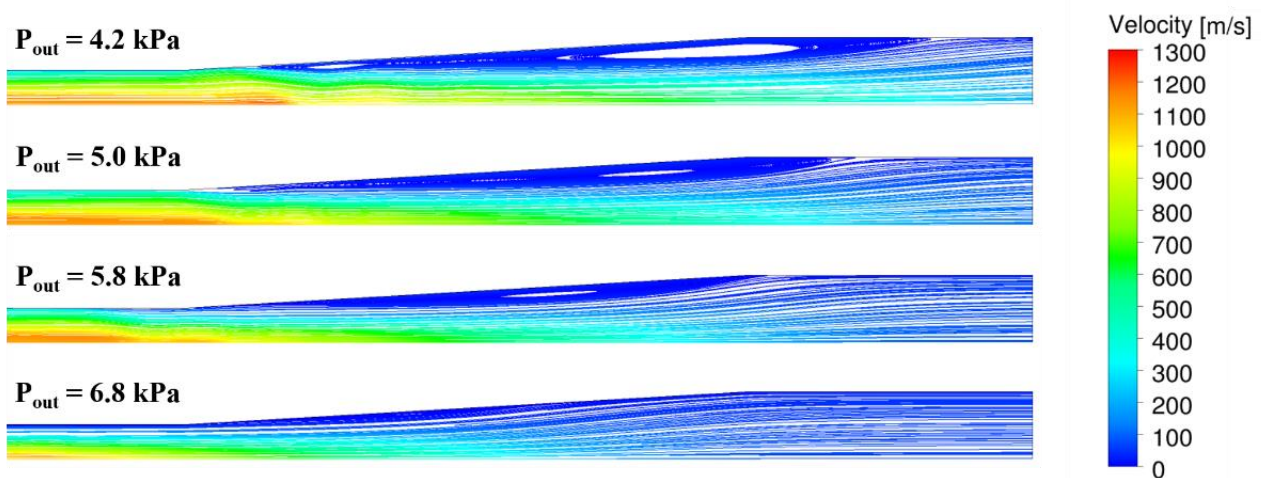
762 Overall, the comparison with experimental data shows a good agreement, especially near the mixing chamber  
763 entrance and throat regions. The accord with experiments decreases as flow approaches the diffuser, where the  
764 recirculations are found. These are notoriously hard to capture by common two-equation turbulence models  
765 and could partly account for the differences with experiments. Furthermore, the discrepancies in the prediction  
766 of the mass flow rates may also impact the results for the pressure trends. This is because the energy budget of  
767 the total stream is altered due to the different proportions of motive and suction flows, changing the positions  
768 of the shock within the diffuser as well as the pressure recovery trends.

769

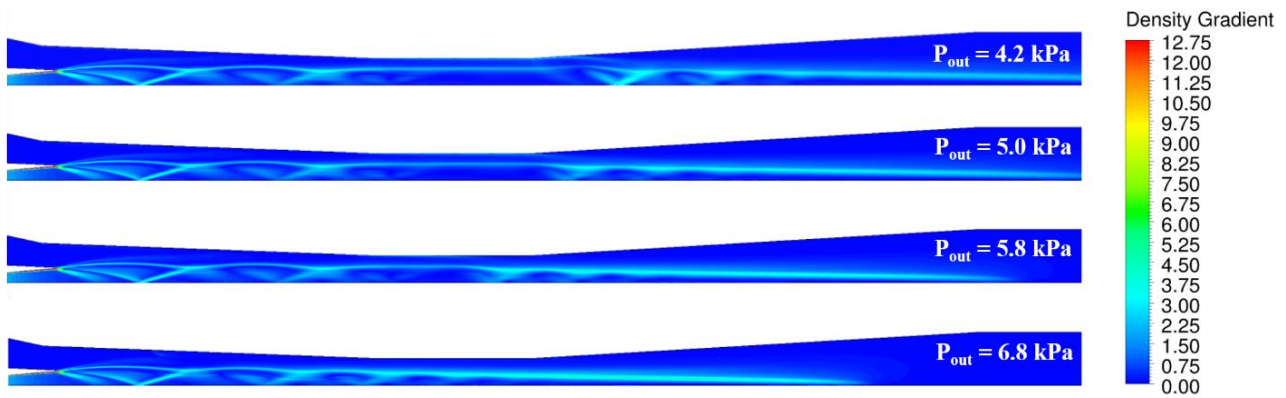


788  
789 *Fig. 10 – Comparison of experimental and numerical wall pressure profiles (experimental data are taken*  
790 *from [9])*

791  
792 [Fig. 11](#) and [Fig. 12](#) show the flow recirculation patterns and shock train structures for the different outlet pressures. It is interesting to note that the case with the lowest outlet pressure present a flow pattern that consists  
793 of two different vortex structures. A first one, smaller, occurs right after the shock train in the diffuser, and a  
794 second, larger, farther downstream. This case also presents the best agreement with the experimental pressure  
795 trend. According to CFD, the patterns adjust to a single vortex structure when the outlet pressure is increased.  
796 However, the agreement with experiments is reduced, therefore, these numerical patterns should be considered  
797 with some caution. Finally, the numerical Schlieren contours in [Fig. 12](#) show that the pressure-based scheme  
798 adopted in this work can qualitatively reproduce the shock train structures within the ejector. However, the  
799 thickness of each shock may be overestimated due to the higher numerical diffusion of these schemes.  
800  
801



802  
803 *Fig. 11 – Streamline pattern at the ejector outlet showing the recirculation regions*  
804

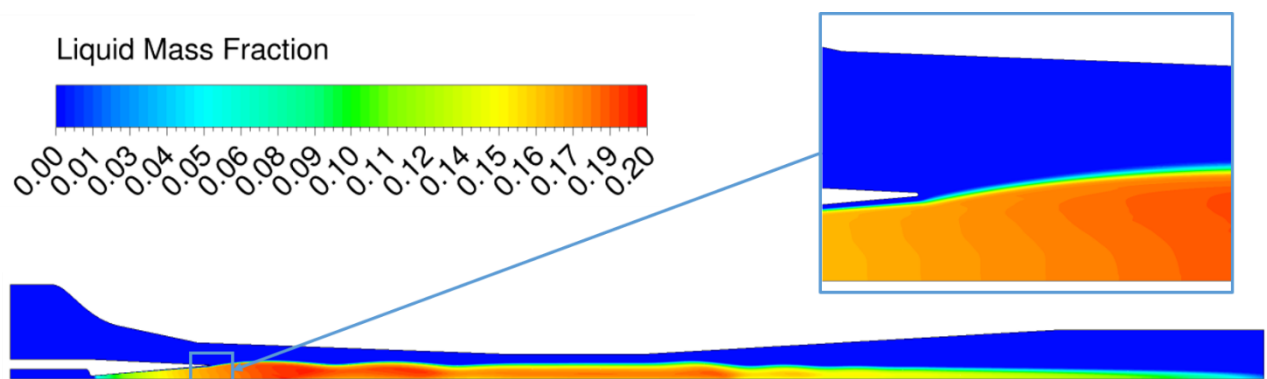


829  
830 *Fig. 12 – Numerical Schlieren images (density gradient contours) showing the shock train structures*  
831

832 ***Two-phase flow features***

833 [Fig. 13](#), shows the contour of the liquid mass fraction for the case with the lowest outlet pressure ( $P_{out} = 4.2$   
834 kPa). As can be seen, the condensed phase reaches value up to 20% of the total mass, with peak levels in the  
835 region downstream of the nozzle exit plane. This is due to the further acceleration caused by the primary jet  
836 under-expansion. The absence of any superheating of the motive stream exacerbate this problem that can lead,  
837 in some extreme cases, to the formation of ice inside the ejector (as discussed in the next section).

838 [Fig. 13](#), further illustrates that the liquid mass fraction evaporates almost completely toward the ejector outlet,  
839 where the mixed stream undergoes the shock trains and decelerate to reach the outlet pressure. In addition, the  
840 liquid mass fraction goes to zero at the nozzle wall, due to the heat recovery caused by the fluid deceleration  
841 and viscous dissipation within the boundary layer [1].  
842



843  
844 *Fig. 13 – Liquid mass fraction contour (case with  $P_{out} = 4.2$  kPa)*  
845

846 [Fig. 14](#), shows the contour of the droplet number per unit mass of mixture,  $n$ . The figure displays also the line  
847 representing the boundary where the liquid mass fraction is zero.

848 The contour clearly reveals the presence of a radial distribution of the droplet number. This stems from the  
849 significant curvature of the nozzle profile at the throat, which induces a region of low pressure near the wall

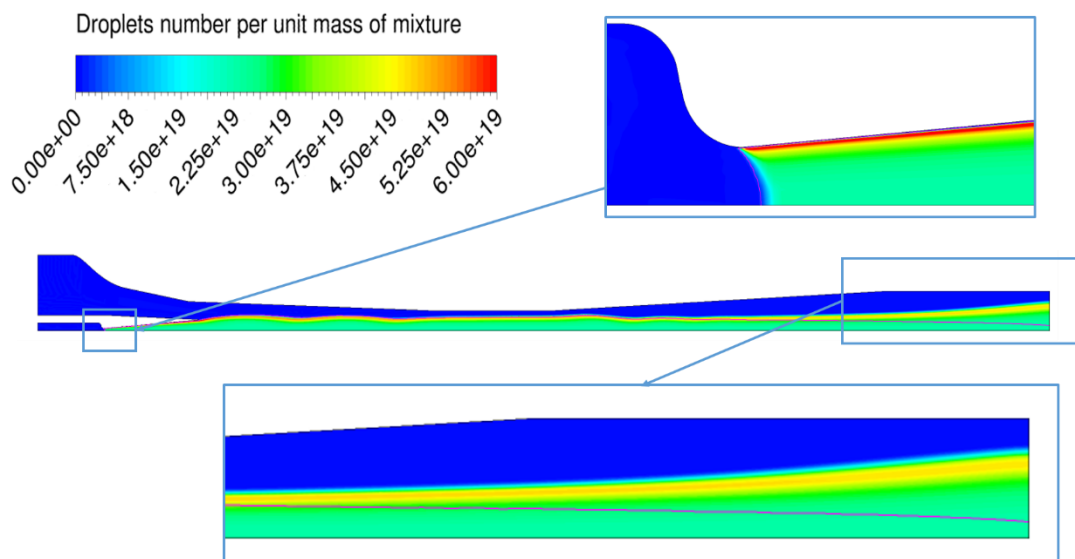
880 and causes a stronger nucleation. The nucleated droplets are then convected down the ejector along streamlines  
881 and the radial distribution persist almost unaltered till the outlet.

882 The analysis of [Fig. 14](#) further shows that the droplets number contour follows closely that of the liquid mass  
883 fraction depicted in [Fig. 13](#). This is a direct consequence of the assumption of equal velocity between the  
884 phases. Yet, the comparison reveals also that toward the ejector outlet, where the condensed mass evaporates  
885 completely, the liquid droplets do not disappear but survive in the form of nuclei with zero mass and volume.  
886 The reason for this numerical error is to be found in the absence of a “droplets sink” term within the droplet  
887 transport equation, eq. (5).

888 This is a common feature of the single-fluid approaches which partly prevent their use in applications where  
889 secondary nucleation occurs (e.g., multi-stage steam turbine cascades). Although in principle it could be  
890 possible to add a sink term to the droplet number equation, in practice, the differential nature of the droplet  
891 transport equation complicates this task. For instance, the inclusion of a negative sink term in eq. (5) leads to  
892 regions with negative numbers of droplets. This problem may be worked around by positively limiting the  
893 value of the droplet number. Unfortunately, this is not possible in ANSYS Fluent.

894 Other options may exist in which, for instance, the value of the sink term is related to the number of droplets  
895 existing in the cell or it is described on a logarithmic basis. To the authors’ knowledge, these approaches have  
896 never been attempted before and may require an extensive development work. However, this effort may not  
897 be completely justified in view of the fact that the assumptions implicit in the single-fluid approach would  
898 anyhow lead to significant approximations (e.g., the droplet sizes originating from different nucleation sites  
899 are averaged out). In this respect, the adoption of more advanced schemes, such as the multi-fluid approach  
900 mentioned in the introduction or a Lagrangian approach (e.g., [32]), naturally account for the removal of  
901 droplets from the computational domain and can provide more accurate results than the method used in this  
902 work.

903



904

905 *Fig. 14 – Contour of the droplet number per unit mass of mixture (in purple is the line where the liquid mass*  
906 *fraction is zero; case with  $P_{out} = 4.2$  kPa)*

936

937 **Model limits**

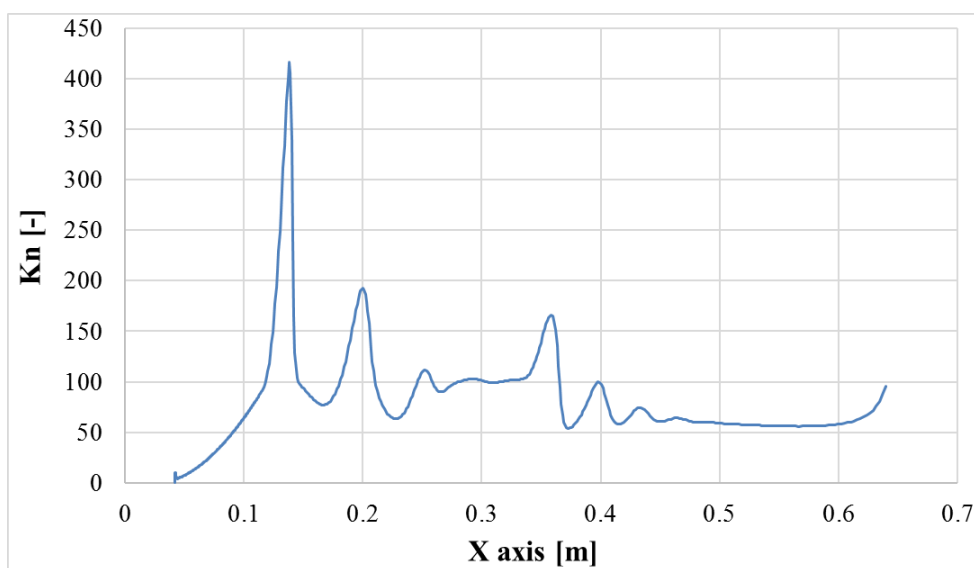
938 In this final section, we would like to review certain specific limits connected with the developed model and  
939 discuss possible implications deriving from them. In doing so, we focus on those assumptions that seem  
940 particularly restrictive with respect to steam ejector applications.

941 A first limit connected with the developed model relates with the droplet growth regime. Generally speaking,  
942 the growth rate formulation for a liquid droplet is calculated differently depending on value of the Knudsen  
943 number. During the initial phase of the droplet growth, the liquid nucleus is generally much smaller than the  
944 mean free path, i.e.,  $Kn \gg 1$ . Under these conditions, named as *free molecular regime*, the continuum  
945 hypothesis does not hold and the calculation of the droplet growth must be accomplished by means of kinetic  
946 theory or statistical mechanics concepts. At the other extreme is the situation where  $Kn \ll 1$ . In this case the  
947 droplet is large enough to apply the macroscopic balances for heat, mass and momentum. In between these  
948 two conditions is what is called the transition regime ( $Kn \sim 1$ ). This is the most difficult to analyze and is usually  
949 handled by means of interpolations formulae that connect the continuum and free molecular regimes (see for  
950 example [18]).

951 Specifically, the Hill's droplet growth law adopted in this work is valid only for the free molecular regime, so  
952 that some questions may arise about its applicability to ejector flows (especially in the case of under-expanded  
953 nozzles with a delayed appearance of shocks that can vaporize or reduce the droplet dimensions [1]).

954 [Fig. 15](#) shows the trend of the Knudsen number along the ejector axis, for one of the simulated cases (but all  
955 cases present similar trends). Clearly, the value of  $Kn$  is always well above unity except for a very small region  
956 near the primary nozzle throat. In this zone, the vapor temperature is still high and the mean free path is of the  
957 same order of magnitude of the droplet diameters (around  $10^{-9}$  m).

958



959 *Fig. 15 – Knudsen number trend along the ejector axis (case with  $P_{out} = 4.2$  kPa)*

960

961

962

Form  
Elimi

994 Somewhat connected with the issue of the droplet growth regime is the assumption of velocity equilibrium  
995 between the phases. In order to understand whether a particle will follow the gaseous stream trajectory or  
996 depart from it, it is possible to estimate the Stokes number related with the particle velocity [39].

997 The Stokes number is defined as the ratio between the droplet response time to a variation in the velocity field  
998 and a flow characteristic time of the continuous phase:

999

$$St = \frac{t_d}{t_v} \quad (19)$$

1000

1001 When the Stokes number is much lower than unity, the condensed phase will closely follow the gaseous stream  
1002 and it is allowed to assume a common velocity between the phases, as in the present work.

1003 The droplet response time depends on the condensed phase inertia and on the carrier phase viscosity [39]:

1004

$$t_d = \frac{\rho_d D_d^2}{18\mu_v} \quad (20)$$

1005

1006 The carrier phase time can be calculated as the ratio between a characteristic velocity and length scale:

1007

$$t_v = \frac{u_v}{L} \quad (21)$$

1008

1009 Clearly, the definition of this last quantity is somewhat arbitrary because no specific definition of the  
1010 characteristic length is provided. For nozzle flow, this is often the throat diameter, the use of which would give  
1011 an estimate of  $St \sim 10^{-3}$ . However, this result refers to a characteristic time representative of the mean flow and  
1012 does not consider any possible velocity mismatch arising from the interaction between turbulence and the  
1013 dispersed phase. To this aim,  $t_v$  can be chosen so as to represent a turbulent characteristic time. Specifically, it  
1014 is possible to calculate the Stokes number by using the inverse of the specific dissipation rate, which represents  
1015 the frequency of the smallest turbulent eddies (those occurring at the Kolmogorov scale), i.e.:

1016

$$t_v = t_{turb\_min} = \frac{1}{\omega} \quad (22)$$

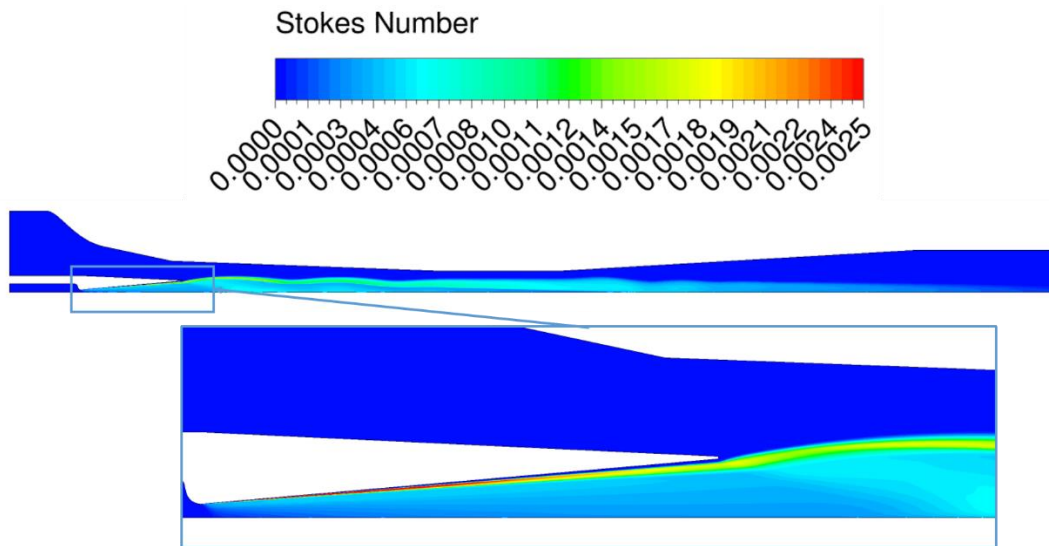
1017

1018 where  $\omega$  is the specific dissipation rate.

1019 [Fig. 16](#) shows a map of this “turbulent” Stokes number within the ejector. Clearly, the assumption of  
1020 equilibrium velocity appears to be satisfied in the whole two-phase flow domain, meaning that the fluid particle  
1021 velocity should follow not only the average flow trajectories, but also the path of the smallest turbulent eddies  
1022 (those with the highest frequency).

1023 However, it should be noted that the above Stokes number was calculated under the assumption of “smooth”  
1024 flow conditions. The presence of any local perturbation may notably reduce the characteristic length, which,

1052 in the specific case of a dynamic shock, is generally of the same order of magnitude of the molecular mean  
 1053 free path. In this case, the different inertia between vapor and liquid droplets may produce a local velocity  
 1054 mismatch and lead to the departure of the phase trajectories. Moreover, the effects of drag and interphase  
 1055 momentum exchange has been neglected in this work although it could represent a non-negligible source of  
 1056 kinetic energy losses. Detailed analyses of these type of processes is a complex task and may require the use  
 1057 of more advanced models than the single-fluid approach.  
 1058



1059  
 1060 *Fig. 16 – “Turbulent” Stokes number within the ejector (case with  $P_{out} = 4.2 \text{ kPa}$ )*  
 1061

1062 Finally, a last, key aspect that is of particular concern for steam ejector studies is related to the very low  
 1063 temperature levels attained by the expanding stream. This problem is particularly critical for ejector  
 1064 refrigeration applications, where efficiency considerations impose the use of low or no level of superheating  
 1065 at the inlet of the motive stream (this is also the case for the experimental results used in this work).  
 1066 Consequently, the motive jet can reach temperature levels that go well below the triple point, causing the  
 1067 possible appearance of ice.

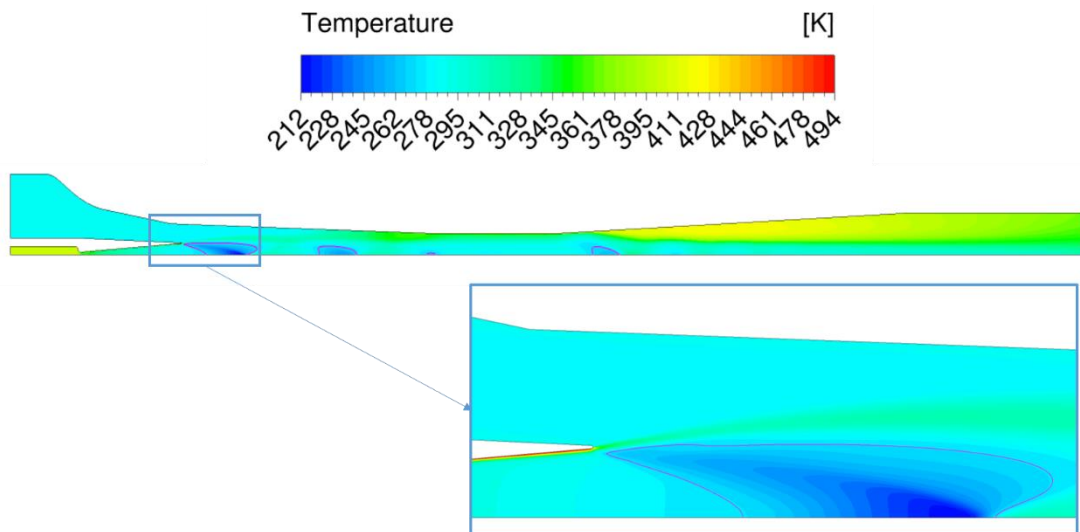
1068 [Fig. 17](#), shows the mixture temperature contour within the ejector. Clearly, the temperature goes well below  
 1069 the limit of the triple point and the presence of ice cannot be excluded (especially downstream of the nozzle  
 1070 exit plane where the mixture temperature reaches values close to 210 K). Nevertheless, ice crystal formation,  
 1071 in much the same way as for droplet nucleation, is fundamentally a time dependent phenomenon and some  
 1072 degrees of supercooling usually exists before the water vapor or liquid starts to solidify.

1073 In particular, experiments in cloud chambers with pure water vapor indicates that the homogeneous nucleation  
 1074 of ice usually occurs with around 30-40 K of supercooling [40]. By contrast, recent investigations in supersonic  
 1075 nozzles have shown that for the high cooling rates and small cluster sizes that are achieved in these devices,  
 1076 the supercooling can be as high as 90 K (i.e., supercooled water temperatures of nearly 190 K) [41]. However,  
 1077 these tests were conducted with ultrapure water and may not be directly applicable to the present study (this is

Form  
 Elim



1079 because impurities in the water droplets or vapor stream can greatly anticipate crystal formation). As a result,  
 1080 the presence of ice cannot be excluded in the steam ejector under investigation.  
 1081 The appearance of water ice crystal may induce substantial modifications to the mixture flow behavior. For  
 1082 instance, the change in the latent heat release (from the value of condensation to that of solidification) may  
 1083 modify the nozzle Mach and pressure profiles. Moreover, phenomena such as crystals agglomeration and  
 1084 deposition may be important and could lead to modifications in the ejector geometrical profiles. On the other  
 1085 hand, the presence of shocks immediately after every steam expansion may lead to the sudden melting of the  
 1086 ice, limiting its impact on the global flow dynamics. In this case, numerical simulations may still incur in  
 1087 significant discrepancies due to the uncertain extrapolation of the supercooled water properties below the triple  
 1088 point temperature (most of these, including viscosity, specific heat, surface tension and others, present  
 1089 exponential variations with decreasing temperatures [40]). In view of these many aspects, it is important that  
 1090 future experimental investigations properly address the analysis of ice formation inside steam ejectors.  
 1091



1092  
 1093 *Fig. 17 – Temperature trend along the ejector; in purple is the line corresponding to the triple point*  
 1094 *temperature (case with  $P_{out} = 4.2$  kPa)*

## 1095 5. Concluding remarks

1096 A numerical model for the simulation of wet-steam flow has been developed and implemented within the CFD  
 1097 software ANSYS Fluent via User Defined Functions. This approach allows great flexibility in the choice of  
 1098 the physical model settings and calibration parameters.

1099 The model has been tested against experimental data from a De-Laval nozzle and a steam ejector test-case.  
 1100 The nozzle simulations have shown that the developed model can produce results that substantially agree with  
 1101 experiments and that are in line with those provided by the ANSYS Fluent wet steam model. However, the  
 1102 model improves on the Fluent built-in scheme by providing a proper conservation of the number of droplets  
 1103 within the computational domain. The analysis of the sensitivity to changes in model settings has shown the  
 1104 importance of both the nucleation rate non-isothermal correction and droplet growth law in predicting the

1105 condensation starting position. By contrast, the adoption of the IAPWS correlation for the surface tension did  
1106 not result in any detectable difference with respect to the formulation used in the present model.  
1107 Simulations for the steam ejector test case have demonstrated a substantial agreement with experiments, both  
1108 in terms of mass flow rates and wall pressure profiles. Some discrepancies are found for the primary mass flow  
1109 rate that probably stems from the presence of liquid at the nozzle inlet or from uncertainties in the nozzle throat  
1110 dimensions. The entrainment of the secondary flow can also be reproduced with accuracy, as long as the effects  
1111 of compressibility on mixing layer development are accounted for in the turbulence model.  
1112 The analysis of the internal flow features has shown that, due to high level of expansion of the primary jet, the  
1113 liquid mass fraction reaches values up to 20% within the mixing chamber. In this region, the mixture  
1114 temperature goes well below the water triple point, indicating the possible presence of ice. However, the  
1115 limited residence time and the presence of shocks may limit the impact of ice formation on the flow dynamics.  
1116 The assessment of the Knudsen and Stokes numbers within the ejector suggests that the approximations of free  
1117 molecular droplet growth regime and velocity equilibrium between the phases should be valid, at least in the  
1118 flow regions away from dynamic shocks.  
1119 In conclusion, it is important to note that some of the most important limitations of the model are related to the  
1120 assumption of the flat-film surface tension as well as to the absence of a sink term in the droplets number  
1121 equation. Improvements in both these two aspects may greatly increase the prediction capability of the wet-  
1122 steam model but require an extensive development and tuning process that will be the subject of future studies.  
1123

## 1124 **References**

1125

- [1] P. P. Wegener and L. M. Mack, "Condensation in Supersonic Wind Tunnels," in *Advances in Applied Mechanics*, New York, Academic Press Inc., 1958, pp. 307-440.
- [2] P. G. Hill, "Condensation of water vapour during supersonic expansion in nozzles," *J. Fluid Mech.*, vol. 25, no. 3, pp. 593-620, 1966.
- [3] J. Starzmann, F. R. Hugues, A. J. White, J. Halama, V. Hric, M. Kolovratnik, H. Lee, L. Sova, M. Statny, S. Schuster, M. Grubel, M. Schatz, D. M. Vogt, P. Y., G. Patel, T. Turunen-Saaresti, V. Gribin, V. Tishchenko, I. Garilov and e. al., "Results of the International Wet Steam Modelling Project," Prague, 2016.
- [4] T. Sriveerakul, S. Aphornratana and K. Chunnanond, "Performance prediction of steam ejector using computational fluid: Part 1. Validation of the CFD results," *International Journal of Thermal Sciences*, vol. 46, pp. 812-822, 2007.
- [5] K. Ariaifar, D. Buttsworth and G. Al-Doori, "Effect of mixing on the performance of wet steam ejectors," *Energy*, vol. 93, pp. 2030-2041, 2015.
- [6] X. Wang, L. H.J., D. J.L. and T. J.Y., "The spontaneously condensing phenomena in a steam-jet pump and its influence," *International Journal of Heat and Mass Transfer*, vol. 55, p. 4682-4687, 2012.
- [7] K. Chunnanond and S. Aphornratana, "An experimental investigation of a steam ejector," *Applied Thermal Engineering*, vol. 24, pp. 311-322, 2004.

- [8] C. A. Moses and G. D. Stein, "On the growth of steam droplets formed in a Laval nozzle using both static pressure and light scattering measurements," *Journal of Fluids Engineering*, pp. 311-322, 1978.
- [9] G. Al-Doori, Investigation of Refrigeration System Steam Ejector Performance Through Experiments and Computational Simulations, Ph.D. thesis, University of Southern Queensland, 2013.
- [10] F. Giacomelli, G. Biferi, F. Mazzelli and A. Milazzo, "CFD modeling of supersonic condensation inside a steam ejector," *Energy Procedia*, no. 101, pp. 1224-1231, 2016.
- [11] A. Gerber and M. Kermani, "A pressure based Eulerian-Eulerian multiphase model for non-equilibrium condensation in transonic steam flow," *International Journal of Heat and Mass Transfer*, pp. 2217-2231, 2004.
- [12] W. Wróblewski, S. Dykas and A. Gepert, "Steam condensing flow modeling in turbine channels," *International Journal of Multiphase Flow*, vol. 35, pp. 498-506, 2009.
- [13] S. Dykas and W. Wróblewski, "Single- and two-fluid models for steam condensing flow modeling," *International Journal of Multiphase Flow*, vol. 37, pp. 1245-1253, 2011.
- [14] C. Brennen, *Cavitation and Bubble Dynamics*, Oxford University Press, 1995.
- [15] F. Bakhtar, J. B. Young, A. J. White and D. A. Simpson, "Classical nucleation theory and its application to condensing steam flow calculations," in *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineers Science*, 2005.
- [16] A. Kantrovitz, "Nucleation in very rapid vapour expansions," *J. Chem. Phys.*, vol. 19, pp. 1097-1100, 1951.
- [17] F. Mazzelli, Single & Two-Phase Supersonic Ejectors for Refrigeration Applications, Florence: Ph.D. Thesis, 2015.
- [18] J. B. Young, "The Spontaneous Condensation in Supersonic Nozzles," *PhysicoChemical Hydrodynamics*, vol. 3, no. 1, pp. 57-82, 1982.
- [19] International Association for the Properties of Water and Steam, "Thermophysical Properties of Metastable Steam and Homogeneous Nucleation," 2011.
- [20] J. B. Young, "An Equation of State for Steam for Turbomachinery and Other Flow Calculations," *Journal of Engineering for Gas Turbines and Power*, vol. 110, no. 1, pp. 1-7, 1988.
- [21] E. Lemmon, M. Huber and M. McLinden, "NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1," 2013.
- [22] ANSYS Inc., *ANSYS Fluent Theory Guide*, Canonsburg, PA: release 18.0, 2016.
- [23] M. Labois and C. Narayanan, "Non-conservative pressure-based compressible formulation for multiphase flows with heat and mass transfer," in *9th International Conference on Multiphase Flow*, May 22nd - 27th, Firenze, Italy, 2016.
- [24] L. Zori and F. Kelecý, "Wet Steam Flow Modeling in a General CFD Flow Solver," in *35th AIAA Fluid Dynamics Conference and Exhibit*, Toronto, Ontario, Canada, 6 - 9 June 2005.
- [25] Y. Yang and S. Shen, "Numerical simulation on non-equilibrium spontaneous condensation," *International Communications in Heat and Mass Transfer*, vol. 36, pp. 902-907, 2009.
- [26] B. Leonard, "A stable and accurate convective modelling procedure based on quadratic upstream interpolation," *Computer Methods in Applied Mechanics and Engineering*, vol. 19, pp. 59-98, 1979.
- [27] G. Gyarmathy, "Bases for a theory for wet steam turbines," PhD thesis, ETH Zurich, 1962.
- [28] M. Joswiak, N. Duff, M. Doherty and B. Peters, "Size-Dependent Surface Free Energy and Tolman-Corrected Droplet Nucleation of TIP4P/2005 Water," *J. Phys. Chem. Lett.*, vol. 4, p. 4267-72, 2013.
- [29] F. R. Menter, "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications," *AIAA Journal*, vol. 32, no. 8, pp. 1598-1605, 1994.

- [30] F. Mazzelli, A. B. Little, S. Garimella and Y. Bartosiewicz, "Computational and Experimental Analysis of Supersonic Air Ejector: Turbulence Modeling and Assessment of 3D Effects," *International Journal of Heat and Fluid Flow*, vol. 56, pp. 305-316, 2015.
- [31] F. Mazzelli and A. Milazzo, "Performance analysis of a supersonic ejector cycle," *International Journal of Refrigeration*, vol. 49, pp. 79-92, 2015.
- [32] F. Hughes, J. Starzmann, A. White and Y. J.B., "A Comparison of Modeling Techniques for Polydispersed Droplet Spectra in Steam Turbines," *Journal of Engineering for Gas Turbines and Power*, vol. 138, 2016.
- [33] H. Ikawa, Turbulent Mixing Layer in Supersonic Flow, Ph.D. thesis, California Institute of Technology, 1973.
- [34] G. Brown and A. Roshko, "On density effects and large structure in turbulent mixing layers," *journal of Fluid Mechanics* , vol. 64, pp. 775-816, 1974.
- [35] A. Smits and J.-P. Dussauge, Turbulent Shear Layers in Supersonic Flow, second edition, New York, NY: Springer, 2006.
- [36] T. Gatsky and J.-P. Bonnet, Compressibility, Turbulence and High Speed Flow, 2nd edition, Oxford, UK.: Academic Press, 2013.
- [37] D. Wilcox, "Dilatation–dissipation corrections for advanced turbulence models," *AIAA Journal*, vol. 11, pp. 2639-2646, 1992.
- [38] D. Wilcox, Turbulence Modeling for CFD, La Canada, California: DCW Industries, Inc, 2006.
- [39] C. Crowe, J. Schwarzkopf, M. Sommerfeld and Y. Tsuji, Multiphase flows with droplets and particles, second edition, Boca Raton, FL: CRC Press, 2012.
- [40] H. R. Pruppacher, "A new look at homogeneous ice nucleation in supercooled water drops," *J. Atmos. Sci.* , vol. 52, pp. 1924-33, 1995.
- [41] J. Wölk, B. Wyslouzil and R. Strey, "Homogeneous nucleation of water: From vapor to supercooled droplets to ice," *AIP Conf. Proc.*, vol. 1527, pp. 55-62, 2013.
- [42] The International Association for the Properties of Water and Steam, "Revised Release on Surface Tension of Ordinary Water Substance," IAPWS report, 2014.

1126

1127