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Comparative evaluation of phase-change mechanisms for the prediction of flashing flows

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Keywords: fuel injectors, two-phase flow, thermodynamic non-equilibrium, kinetic theory of gases, Homogeneous Relaxation Model, bubble dynamics

Abstract. A numerical study is presented, evaluating in a comparative manner the capability of various mass-transfer rate models to predict the evolution of flashing flow in various geometrical configurations. The examined models comprise phase-change mechanisms based on the kinetic theory of gases (Hertz-Knudsen equation), thermodynamic-equilibrium conditions (HEM), bubble-dynamics considerations using the Zwart-Gerber-Belamri model (ZGB), as well as semi-empirical correlations calibrated specifically for flash boiling (HRM). Benchmark geometrical layouts, i.e a converging-diverging nozzle, an abruptly contracting (throttle) nozzle and a highly-pressurized pipe, for which experimental data are available in the literature have been employed for the validation of the numerical predictions. Consideration on additional aspects associated with phase-change processes, such as the distribution of activated nucleation sites, as well as the deviation from thermodynamic-equilibrium conditions have also been taken into account. The numerical results have demonstrated that the onset of flashing flow in all cases is associated with the occurrence of compressible flow phenomena, such as flow choking at the constriction location and expansion downstream, accompanied by the formation of shockwaves. Phase-change models based on the kinetic theory of gases produced more accurate predictions for all the cases investigated, while the validity of the HRM and ZGB models was found to be situational. Furthermore, it has been established that the inter-dependence between intrinsic physical factors associated with flash boiling, such as the nucleation-site density and the phase-change rate, has a significant, yet not clearly distinguishable influence on the two-phase flow characteristics.

46		
47	Nomenclature	
48	A	area [m ²]
49	a	volume fraction [-]
50	c	sonic velocity [m/s]
51	C _{evap}	empirical coefficient
52	c _p	specific heat at constant pressure [J/kgK]
53	c _v	specific heat at constant volume [J/kgK]
54	D	diffusion coefficient [m ² /s]
55	F _e	coefficient of the ZGB model
56	h	specific enthalpy [J/kg]
57	k	thermal conductivity [W/mK]
58	Le	Lewis number, $Le = k/\rho D c_p$
59	M	Mach number, $M = u/c$ [-]
60	N _b	nucleation-site density [sites/m ⁻³]
61	p	pressure [Pa]
62	R	evaporation rate [kg/m ³ s]
63	R _b	bubble radius [m]
64	R _g	ideal gas constant [J/Kmol]
65	T	temperature [K]
66	Sc	Schmidt number, $Sc = \mu/\rho D$
67	t	time [s]
68	u	velocity [m/s]
69	Y	mass fraction [-]
70	<i>Greek letters</i>	
71	Θ _r	fraction relaxation time [s]
72	λ	accommodation coefficient [-]
73	μ	viscosity [kg/ms]
74	ρ	density [kg/m ³]
75	<i>Subscripts/Abbreviations</i>	
76	crit	critical
77	e	equilibrium
78	GDI	Gasoline Direct Injection
79	HK	Hertz-Knudsen
80	HEM	Homogeneous Equilibrium Model
81	int	interphase
82	i	phase
83	l	liquid
84	mix	mixture
85	nuc	nucleation
86	sat	saturation
87	sup	superheat
88	t	turbulent
89	v	vapour

90 vof volume fraction

91

92 **1. Introduction**

93 The main objective of modern engine-components manufacturers is to produce
94 environmentally friendly IC engines, so as to be in compliance with the ever stricter pollutant-
95 emissions legislations imposed globally. Along these lines, significant research effort has been
96 made over the past years for the development of efficient fuel injectors producing an atomized
97 spray of high quality, which, in turn, designates the combustion efficiency. It has been
98 established in the literature that apart from increasing the injection pressure, enhancement of the
99 spray-atomization efficiency can be accomplished by increasing the fuel temperature (Sens et al.,
100 2012). Besides, the topology and evolution of the two-phase jet exiting the injector have been
101 found to be in strong correlation to the in-nozzle flow conditions and primarily to the phase-
102 change rate (Karathanassis et al., 2016). Flash boiling (flashing) is a phase-change process
103 manifested through vapour production due to a rapid liquid depressurization forcing the liquid
104 saturation temperature to values lower than the local liquid temperature; this temperature
105 difference being termed as liquid superheat. The process can be characterized as thermally
106 driven, since the rate of bubble growth is designated by the heat transfer rate at the bubble
107 interface.

108 There is a significant number of studies available in the literature referring to flashing spray
109 flows. Initial studies, as well as more recent experimental investigations, have employed front or
110 back-lighting projection (shadowgraphy or Schlieren) methods to qualitatively characterize the
111 spray quality (Oza, 1984; Reitz, 1990; Vieira and Simões-Moreira, 2007; Lamanna, 2014).
112 Fundamental studies focusing on identifying the complex flow topology in the near-nozzle
113 region have been performed in simple-orifice geometries and have revealed flow choking at the
114 nozzle outlet and downstream expansion leading to supersonic velocities, increased spray cone
115 angle and formation of shockwaves (Vieira and Simões-Moreira, 2007). The experimental
116 investigation performed by Lamanna et al. (2014) has highlighted that the topology of the spray
117 exiting the nozzle is controlled by bubble nucleation upstream of the nozzle outlet.

118 Referring to practical applications associated with automotive engineering, the vast majority
119 of experimental studies also focuses on visualizing the external spray region, with the main
120 interest being in GDI-engine injector layouts, which are possible to operate under flash boiling
121 conditions. The high-speed shadowgraphy study of Serras-Pereira et al. (2010) provided
122 simultaneous visualization in the in-nozzle and spray regions of a single-hole injector and
123 demonstrated that lightweight-fuel (gasoline, n-pentane) sprays characterized by a high degree of
124 superheat were found to comprise a high concentration of vapour and fine droplets within the
125 spray. Especially for n-pentane, it was found that the jet emerged already atomized at the nozzle
126 outlet. A subsequent, experimental investigation conducted by Aleiferis and van Romunde
127 (2013) regarding a multi-hole gasoline injector with heated fuel revealed that convergence
128 (collapse) of the different plumes into a single one occurred when the droplet size decreased
129 below 12 μm . Optical, flow-visualization techniques have been widely used for the
130 determination of the macroscopic features of flashing sprays, such as spray-cone angle and tip
131 penetration (Araneo et al., 2000; Mojtabi et al., 2008; Chan 2014). It has been established that
132 onset of flash boiling conditions is associated with reduced spray penetration and increased
133 spray-cone angle.

134 Further laser-diagnostics studies employing the Laser Induced Exciplex Fluorescence (LIEF)
135 technique, according to which the fluorescence of two laser-excited dyes added to the base fuel is

136 proportional to the liquid and vapour phase fraction, have been used for the elucidation of
137 flashing sprays, considering the effects of both fuel temperature and ambient pressure (Payri et
138 al., 2006; Zhang et al., 2012; Zeng et al., 2012;). Zhang et al. (2012) reported that for a gasoline
139 surrogate (n-hexane) and a superheat degree of 30K, the LIEF visualization showed significant
140 vapour production in the spray region signifying the plume collapse to a single structure. Zeng et
141 al. (2012), in his LIEF visualization of the spray emerging from a gasoline multi-hole injector
142 distinguished two separate flashing regimes based on the collapse of the different spray plumes.
143 It was concluded that the spray macroscopical features, i.e. penetration and cone angle exhibited
144 inverse trends in the two flashing regimes, i.e. prior and after the collapse of the plumes.

145 Besides, a number of numerical investigations have been performed regarding flashing flows
146 associated with fuel-injection equipment, with once again the main interest being in externally
147 flashing meta-stable liquid jets. Different phase-change models based on the degree of liquid
148 superheat have been proposed for the vaporization of a flashing spray being expelled into a
149 gaseous environment (see selectively Zuo et al. (2000) and Price et al. (2015)), which have been
150 found to produce accurate predictions regarding the spray macroscopic features, i.e. penetration
151 and plume width. The numerical studies have also confirmed the trend of increased vapour
152 production at elevated fuel temperatures.

153 On the contrary, limited modelling approaches have been proposed in the literature in
154 reference to geometrically confined flows. Liao and Lucas (2015) modelled the flashing flow in
155 a venturi nozzle, considering that the phase-change rate is dependent on the heat transfer at the
156 bubble interface. Analytical correlations based on the Peclet and Jakob numbers were used for
157 the determination of the local heat transfer coefficient. Schmidt et al. (2010) employed the
158 Homogeneous Relaxation Model (HRM) for the prediction of flashing in steady channel flows.
159 Their numerical predictions showed good agreement with the available experimental results. The
160 HRM model has also been employed in a number of studies to simulate flashing flow in various
161 nozzle geometries and fuels ranging from swirl atomizers to jet-engine applications (Lee et al.,
162 2009; Gopalakrishnan and Schmidt, 2008; Neroorkar et al., 2011). It must be noted that the
163 HRM model has been deemed suitable even for the numerical prediction of cavitating flows due
164 to the similar macroscopic manifestation of the two phenomena (Battistoni et al., 2014). In a
165 recent publication, Saha et al. (2016) coupled the HRM model to the VOF method, in order to
166 predict the in-and near-nozzle two-phase flow evolution of a real GDI injector (Engine
167 Combustion Network, 2014) under realistic operating conditions. The numerical results allowed
168 the distinction of two external vaporization regimes corresponding to flash boiling and
169 convective vaporization owing to the high temperature of the gas medium, where the jet was
170 expelled into.

171 Although the aforementioned experimental investigations have demonstrated the connection
172 between the in- and near-nozzle two-phase flow, from a numerical perspective, there are only
173 limited studies in the literature elucidating the in-nozzle phase-change mechanism, the factors
174 that have an influence on it, as well as its after-effects on the flow pattern at the near-field region.
175 The present study serves as a comparative evaluation of the predictive capability of various
176 mass-transfer mechanisms (kinetic theory of gases, bubble dynamics, equilibrium and non-
177 equilibrium, semi-empirical) in capturing the phase change in nozzle and pipe flashing flows.
178 Besides, it aims to elucidate the importance of the various model parameters, reflecting intrinsic
179 physical quantities, such as the distribution of nucleation sites or the conditions at the bubble
180 interface, on the designation of the overall phase-change rate. The link between the phase-change
181 rate and the velocity and pressure fields is identified and thoroughly explained, allowing the

182 justification of distinct flow phenomena associated with flashing flows, including, increase of the
183 spray-cone angle and formation of shockwaves. The formulation of the numerical models is
184 discussed in detail in the next section, followed by the presentation of the numerical predictions.
185 The main findings of the study are summarized in the conclusions section.

186 **2. Description of the cases investigated**

187 *2.1 Benchmark geometries and operating conditions*

188 Three geometrical arrangements have been selected for performing numerical simulations.
189 The relatively simple geometries used ensure that no significant flow perturbations induced by
190 the geometrical layout will set in. In addition, experimental data are available for all the cases
191 examined, allowing the verification of the numerical-predictions validity. More specifically, the
192 benchmark geometries comprise a convergent-divergent nozzle (“Moby Dick” nozzle) (Asaka,
193 1992; Staedtke, 2006), a throttle-nozzle with an abrupt decrease of its cross section used in the
194 experimental investigation of Reitz (1990), as well as a highly-pressurized pipe (Edwards’ blow-
195 down pipe) (Edwards and O’Brien, 1970). In terms of flow conditions, the first two cases
196 constitute steady inlet-outlet flows, while in the “Edwards’ pipe” case, the phase-change process
197 is transient and leads to full vaporization of the liquid. Water was used as the working medium in
198 all configurations with variable thermophysical properties calculated through the respective
199 values available in the IAPWS tables (Wagner and Pruss, 2002).

200 The total length of the “Moby Dick” nozzle, shown in **Fig. 1a**, is approximately equal to 1.0m
201 and comprises a convergent section, a long cylindrical throat and a divergent section with an
202 angle of aperture of 7° . The nozzle is operating with inlet and outlet pressures equal to 20.0bar
203 and 5.0bar respectively, with the liquid temperature at the inlet being 2.0 K lower than the
204 saturation temperature for the prevailing pressure. The “Reitz” nozzle depicted in **Fig. 1b**
205 realizes a step-wise flow contraction with a blockage ratio (D_{down}/D_{up}) of 4.65, whereas the
206 nozzle length to diameter ratio is equal to 4. A constant pressure equal to 7.88bar, is set at the
207 nozzle inlet, while the flow discharge is straight to the environment. Different test-cases were
208 examined by Reitz (1990) with the liquid temperature being in the range 360-427K. **Fig. 1c**
209 depicts the schematic representing the “Edwards’ pipe”, a duct with a length of approximately
210 4.0m containing water pressurized at 7.0MPa through a disc placed at its outlet and temperature
211 of 502K. The transient blow-down is initiated by the rupture of the disk allowing the rapid
212 discharge to the environment at atmospheric pressure.

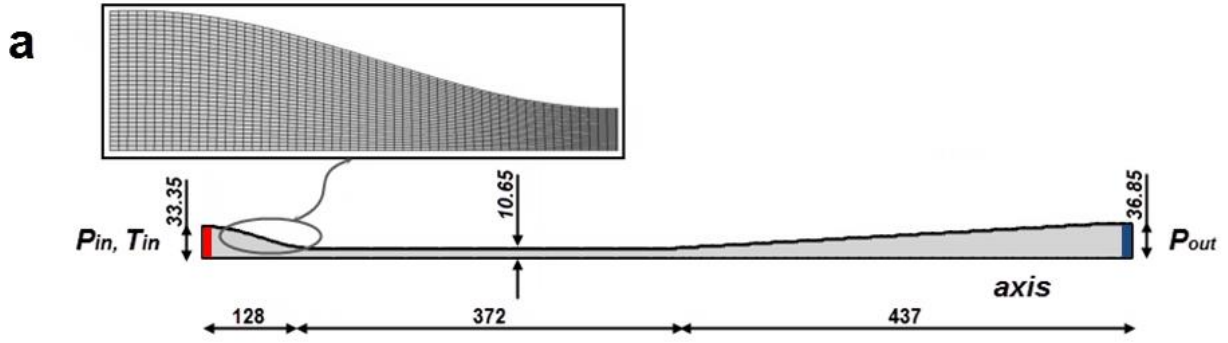
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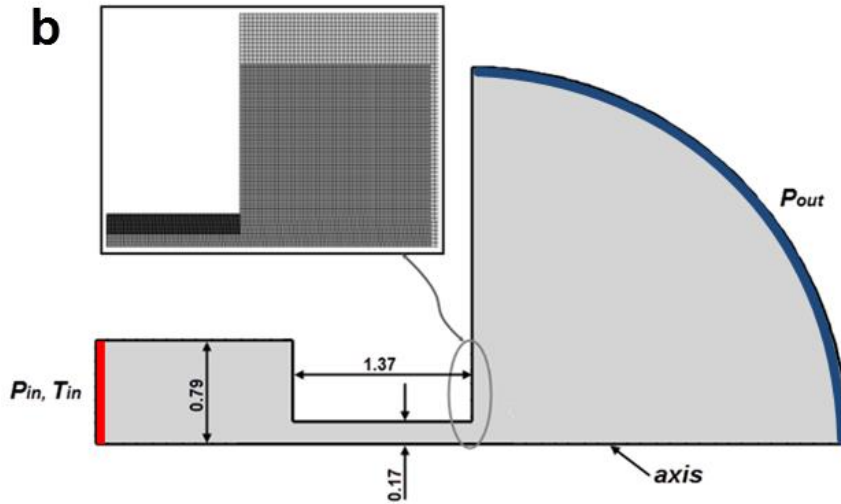
215 *2.2 Computational domains and governing equations*

216 Since all the nozzle layouts considered are axisymmetric, two-dimensional domains were
217 deemed as representative of the actual geometries and were used for the simulations (**Fig. 1**). It
218 must be noted that the domains were extended and appropriate volumes were placed at the outlet
219 regions of the “Reitz” and “Edwards” cases, so that boundary conditions are not placed in
220 regions, where high gradients are expected to occur and, furthermore, to allow the un-perturbed
221 evolution of the jet cone downstream the geometrical constriction. Domain discretization was
222 performed using primarily structured grids, as also depicted in **Fig. 1**. Telescopic, local grid
223 refinement methodology allowed the creation of a fine grid in the regions, where complex flow
224 phenomena are expected to occur, e.g. at the regions of flow contraction/expansion.

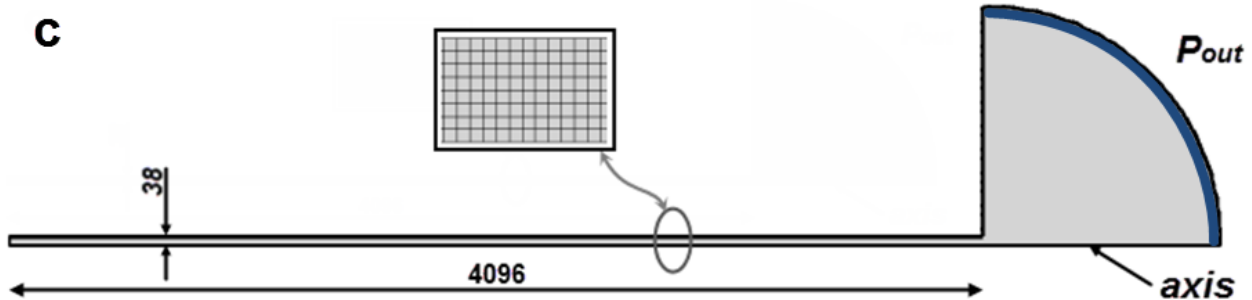
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Figure 1. Computational domain and grid topology (all dimensions in mm): (a) “Moby Dick” nozzle, (b) “Reitz” nozzle, (c) “Edwards’ pipe”.

A two-phase mixture model was employed in order to capture phase-change effects with a common velocity field assumed for the two phases (mechanical-equilibrium assumption). The liquid phase was treated as compressible (Tait equation of state), while the respective vapour phase was considered an ideal gas. The set of governing equations comprised the continuity, momentum and energy equations for the two-phase mixture (ANSYS FLUENT, 2012), as well as an additional advection equation corresponding to the conservation of the secondary phase, i.e. the vapour, volume fraction α :

$$240 \quad \frac{\partial(\rho_{mix})}{\partial t} + \nabla(\rho_{mix}\vec{u}) = 0 \quad (continuity)$$

241 (1a)

$$242 \quad \frac{\partial(\rho_{mix}\vec{u})}{\partial t} + \nabla(\rho_{mix}\vec{u}\vec{u}) = -\nabla p + \nabla[\mu_{mix}(\nabla\vec{u} + \nabla\vec{u}^T)] \quad (momentum) \quad (1b)$$

244

$$245 \quad \frac{\partial}{\partial t} \sum_{i=1}^2 (a_i \rho_i E_i) + \nabla \sum_{i=1}^2 (a_i \vec{u} (\rho_i E_i + p)) = \nabla(k_{mix} \nabla T), \quad E_i = h_i - \frac{p}{\rho_i} + \frac{u_i^2}{2} \quad (energy)$$

246 (1c)

$$247 \quad \frac{\partial(a\rho_v)}{\partial t} + \nabla(a\rho_v\vec{u}) = \dot{R} \quad (vapour\ volume\ fraction) \quad (1d)$$

249 where the indices *mix* and *i* correspond to the mixture and each separate phase. Referring to **Eqs.**
 250 **(1a)-(1d)** ρ , h , α , \vec{u} , \dot{R} correspond to density, sensible enthalpy, vapour volume fraction,
 251 velocity field and vaporization mass-transfer rate. Especially referring to the energy **Eq. (1c)**,
 252 further details on the definition of the internal energy and the numerical manipulation performed
 253 by the commercial solver can be found in (ANSYS FLUENT, 2012). The modelling approach
 254 according to which an additional vapour volume-fraction conservation equation, **Eq. (1d)**, is
 255 solved, with a source term added to its right-hand side to account for liquid vaporization
 256 constitutes common practice in reference to two-phase flows (see selectively, Magnini and
 257 Pulvirenti, 2011; Lee et al., 2009; Janet et al., 2015; Ji et al., 2014; Yan et al., 2001; Žnidarčič et
 258 al., 2015). The addition of a diffusion term of the form $(\rho D + \frac{\mu_t}{Sc}) \nabla Y$ on the right-hand side of
 259 **Eq. (1d)** has been verified through preliminary simulations performed for the Moby-Dick case,
 260 assuming a constant, approximate value for the diffusion coefficient $D(=k/\rho c_p \approx 10^{-7} \text{ m}^2/\text{s}$, i.e.,
 261 $Le=1$) and $Sc=0.7$, to have a negligible effect on the produced numerical results. Hence, taking
 262 into account that the main objective of the present study is to compare different phase-change
 263 rates for flashing flows, and that data are not available for D in reference to such flows, **Eq. (1d)**
 264 has been employed in the presented form. Yet depending on the prevailing flow conditions, the
 265 effect of the diffusion term could be significant and should not be omitted referring to other two-
 266 phase flows not relevant to this study.

267 It must be pointed out that contributions to the mixture viscosity μ_{mix} and thermal conductivity
 268 k_{mix} are made by terms specified using the k- ω SST model to account for turbulence effects, as
 269 the nominal Reynolds-number values characterizing the flow in the “Moby Dick”, “Reitz” and
 270 “Edwards’ pipe” cases are in the order of $4.0 \cdot 10^6$, 62000 and, 10^7 respectively, which are well
 271 within the turbulent regime. The SST k- ω model was selected to capture turbulence effects, as it
 272 has been demonstrated to be performing well to both moderately and highly turbulent flows, and
 273 furthermore it is recommended for flows where recirculation is possible to set in, e.g. throttle
 274 flows (Menter, 2012).

275 As also depicted in **Fig. 1**, suitable boundary conditions were supplied for the governing
 276 equations, in order to numerically replicate the flow conditions prevailing during the respective
 277 experimental investigations. Constant pressure values, equal to the operating ones set during the
 278 experiments, were imposed at the domain inlet and outlet for the “Moby Dick” and “Reitz”

279 computational domains. A constant inlet temperature of 483.5K was set for the “Moby Dick”
280 nozzle, while inlet temperatures in the range 400-427K, as onset of flash boiling was detected for
281 the specific range, were set for the different test cases examined for the “Reitz” nozzle.
282 Regarding the “Edwards’ pipe” domain, a constant atmospheric pressure was imposed at the
283 outlet, i.e. at the edge of the quarter-circular plume. All the other outer edges of all three
284 domains, apart from the axis of rotation, were treated as walls and the no-slip condition was
285 imposed.

286 The “Moby Dick” and “Reitz” simulations were initialized assuming pure liquid in the entire
287 domain, while the pressure was set equal to the inlet pressure. Especially for the HRM (see
288 section 2.3), where a non-zero value of a is required for phase change to commence, initial
289 values of $p=p_{out}$ and $a=1$ were patched at the expanding parts of the aforementioned domains,
290 since preliminary simulations verified full vaporization and depressurization of the liquid at
291 those regions. For the “Edwards’ pipe” case, in order the transient phenomenon to commence
292 pure liquid ($a=0$) must be assumed within the duct ($X<4096mm$) and pure vapour ($a=1$) at the
293 duct outlet and downstream ($X\geq 4096mm$). Calculations for the first two cases were carried out
294 until it was confirmed that a steady solution had been reached and it was verified that a flow time
295 of 2.5 ms was sufficient for both cases. The simulation was declared as complete for the
296 “Edwards’ pipe” case after a total flow time of 0.5s for which the entire liquid within the duct
297 had been fully vaporized.

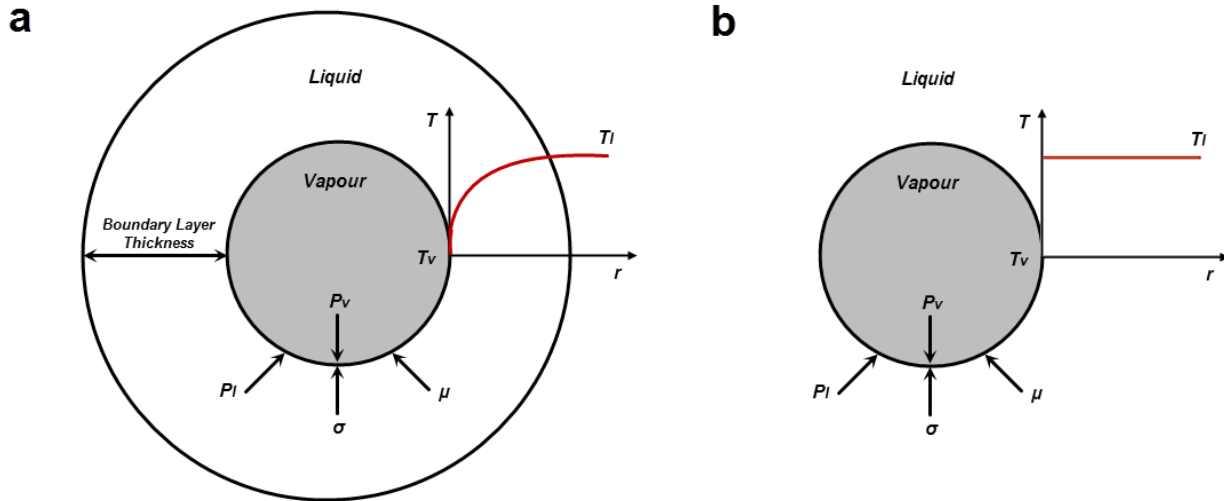
298 The coupled pressure/velocity, implicit solver implemented in FLUENT (v. 14.5) (2012) was
299 used, with second order schemes for turbulence advection and momentum. The capability of
300 coupled solvers to predict compressible/shockwave flows has been demonstrated in the literature,
301 see selectively (Demirdžić et al., 1993; Chen and Przekwas, 2010; Koukouvinis and Gavaises,
302 2015). The transient solver was employed with a time step of $1\cdot 10^{-6}$ s, which produced values of
303 the Courant–Friedrichs–Lewy (CFL) condition less than 15 for all cases that can be easily
304 handled by the implicit solver. It must be noted that 15 corresponds to the maximum cell CFL
305 value obtained for all the cases examined. The specific value occurred at the throttle region of
306 the “Reitz” configuration where the grid is very fine (see **Fig. 1b**) and high flow velocities occur.
307 However, the flow in both the “Moby Dick” and “Reitz” cases converges to steady-state
308 solutions, and hence relatively high CFL values do not interfere with the solver capability of
309 capturing phenomena associated with compressible flow, such as shockwaves, the occurrence
310 location of which remains static and time-invariant in the aforementioned cases. Referring to the
311 “Edwards’ pipe” layout, where the flow is transient, the time step has been properly adjusted, so
312 as the Courant number not to exceed a value of 0.8 throughout the evolution of the solution.
313 Although, the flow reaches a steady-state solution in the “Moby Dick” and Reitz cases, yet the
314 transient solver was employed in order to improve the convergence of the solution.

315
316

317 *2.3 Two-phase/Mass-transfer models*

318 From a flow physics point of view, the discrimination between equilibrium and non-
319 equilibrium conditions refers to the temperature distribution locally at the interface between the
320 growing bubble and the surrounding interface. At equilibrium conditions, a thermal boundary
321 layer of non-negligible thickness (see **Fig. 2a**) surrounds the bubble interface and hence the
322 liquid and vapour temperature on each side of it are postulated as equal. Consequently, heat
323 transfer rate is infinite and the phase-change process is governed by inertia. On the contrary, for
324 non-equilibrium conditions (**Fig. 2b**) the boundary layer thickness is taken as infinitesimally

325 small and a temperature discontinuity occurs at the interface. In that case, the bubble-interface
 326 velocity and consequently the phase-change rate are strongly linked to the finite local heat
 327 transfer rate designated by the respective temperature gradient.
 328



329
 330
 331 **Figure 2.** Schematic of growing bubble and surrounding liquid for thermodynamic (a)
 332 equilibrium and (b) non-equilibrium conditions.
 333

334 In the framework of the present investigation, a number of approaches were considered for
 335 modelling the mass-transfer rate term of Eq. (1c) by also taking into account non-equilibrium
 336 phenomena. The phase-change models formulated in this section were implemented in the solver
 337 as User Defined Functions (UDFs). Firstly, a generalized mass-transfer rate derived from kinetic
 338 theory of gases and similar to the initial correlation proposed by Knudsen (1915) has been tested:
 339

$$340 \quad \dot{R} = C_{evap} A_{int} a_l \rho_l (p_{sat} - p) \quad (2)$$

341 where a_l and ρ_l are the liquid volume fraction and density, respectively, while C_{evap} is an
 342 empirical coefficient. A correction has been made to the saturation pressure, namely
 343 $p_{sat} = p_{sat}(T) + \frac{1}{2}(0.39k\rho)$, with k being the turbulent kinetic energy, in order to take into account
 344 the effect of turbulence on cavitation inception as reported, for instance by Singhal et al. (2002).
 345 The mentioned correction has been applied to all two-phase models. A_{int} is the overall bubble-
 346 cloud interphase surface area, which is calculated assuming a nucleation-site density of 10^{13}
 347 sites/m³ and a bubble radius of 10^{-6} m. It has to be pointed out that, since the mixture model is
 348 employed, the bubble interface is not captured and therefore the bubble-cloud distribution is, in
 349 essence, a “lumped” parameter employed for the determination of the overall phase-change rate.
 350 The assignment of a constant distribution of vapour bubbles, of course, constitutes an
 351 approximation, however it is essential to bear in mind that contaminants, micro-bubbles or
 352 impurities, in the bulk of the liquid act as potential nucleation sites and hence the determination
 353 of the actual distribution is actually case dependent. It has been verified by different water-tunnel
 354 experiments that the nucleation-site density in the case of cavitating flow lies within the range
 355

356 10^{12} - 10^{13} sites/m³ for vapour bubbles having radii less than 10 μ m, as summarized by Brennen
 357 (1995). The measurements of Ceccio (1990) regarding cavitation development over a benchmark
 358 protrusion also verified a site density approximately equal to 10^{12} for bubbles with radii of 10 μ m.
 359 Zwart et al. (2004) have calibrated their phase-change model at several benchmark cases and
 360 deduced that a bubble radius of 1 μ m offers the best matching to available experimental data. To
 361 the authors' knowledge there are no data for the nucleation site distribution available in the
 362 literature, in reference specifically to flashing flows. However, estimations derived through
 363 numerical models are in the range of 10^9 - 10^{11} sites/m³ considering bubble radii of the order of
 364 10 μ m (Riznic and Ishii, 1989; Shin and Jones, 1993). Based on the above, a distribution of 10^{13}
 365 bubbles per m³ of liquid with radii of 1 μ m has been adopted in the present study, which
 366 produces an overall interphase surface area comparable to the available data for both cavitating
 367 and flashing flows, while also the bubble-radius value employed is in compliance with that
 368 suggested by Zwart et al. (2004).

369 A variation of the Hertz-Knudsen equation (Fuster et al., 2010), where deviation from
 370 thermodynamic-equilibrium conditions is taken into account through an accommodation
 371 coefficient λ , has also been considered:

$$372 \dot{R} = \frac{\lambda A_{int} (p_{sat} - p)}{\sqrt{2\pi R_g T_{int}}} \quad (3)$$

374 where R_g and T_{int} are the ideal gas constant and the temperature at the bubble interphase,
 375 respectively. As has been already discussed, an interphase-capturing technique is not employed
 376 in the present study; consequently, the interphase temperature is taken as equal to the local cell
 377 temperature, which is calculated by the solution of the energy equation. A value of unity for the
 378 λ coefficient corresponds to a heat-transfer rate at the bubble interphase approaching infinity and
 379 thus thermodynamic-equilibrium conditions. On the contrary, a value of 0.1 or lower suggests a
 380 significant deviation from equilibrium (Brennen, 1995). A different formulation of Eq. (3) where
 381 a temperature discontinuity is assumed at the bubble interface, as proposed by Theofanous et al.
 382 (1969), has also been considered:

$$383 \dot{R} = \frac{\lambda A_{int}}{\sqrt{2\pi R_g}} \left(\frac{p_{sat}}{\sqrt{T_l}} - \frac{p}{\sqrt{T_v}} \right) \quad (4)$$

385 with T_l and T_v being the local liquid and vapour temperature, respectively, with the latter being
 386 taken equal to the saturation temperature for the local pressure.

387 The Homogeneous Relaxation Model (HRM) (Bilicki and Kestin, 1990) has also been
 388 proposed as suitable for the prediction of flashing flow and is based on the concept that thermal
 389 equilibrium between the liquid and vapour phases establishes after the passage of a characteristic
 390 time interval referred to as fraction relaxation time Θ_r given by the following relation:

$$391 \Theta_r = \Theta a^m \phi^n \quad (5)$$

394

395 where Θ is a semi-empirical timescale, m and n are fitting coefficients, a is the vapour volume
 396 fraction and ϕ is a non-dimensional pressure difference defined as:

$$397 \phi = \left| \frac{p_{sat} - p}{p_{sat}} \right| \quad (6a)$$

399 for pressures below 10 bar, whereas for pressures exceeding that value, the following correlation
 400 has been proposed:

$$401 \phi = \left| \frac{p_{sat} - p}{p_{crit} - p_{sat}} \right| \quad (6b)$$

402
 403 Indicative values for Θ_0 , m and n , as reported by Schmidt et al. (2010), are $6.51 \cdot 10^{-4}$ s, -0.257,
 404 and -2.24, for the “low pressure” formulation of the model ($p < 10$ bar), whereas for the
 405 respective “high-pressure” variation, the corresponding values are $3.84 \cdot 10^{-7}$ s, -0.54, and -1.76.
 406 The mass-transfer rate then results as:

$$407 \dot{R} = -\rho_{mix} \frac{Y - Y_e}{\Theta} \quad (7)$$

408 where ρ_{mix} is the mixture density and Y_e is the thermal-equilibrium mass fraction calculated using
 409 the following relation:

$$410 Y_e = \frac{h_{mix} - h_{sat,l}}{h_{sat,v} - h_{sat,l}} \quad (8)$$

411 where h_{mix} corresponds to the mixture specific enthalpy, while $h_{sat,v}$, $h_{sat,l}$ are the vapour and
 412 liquid specific enthalpies at saturated conditions.

413 Finally, considering that cavitation and flash boiling could be characterized as processes of
 414 similar nature, since both are manifested through bubble nucleation caused by a rapid
 415 depressurization process, a bubble-dynamics model has also been taken into account for the
 416 present investigation. The model proposed by Zwart et al. (ZGB model) (2004) is based on the
 417 solution of a simplified form of the Rayleigh-Plesset equation, where the higher order, viscosity
 418 surface tension and gas content terms are neglected. Semi-empirical parameters are also
 419 employed by the model in order the mass-transfer rate to be derived:

$$420 \dot{R} = F_e \frac{3a_{nuc}a_l}{R_b} \sqrt{\frac{2}{3\rho_l} (p_{sat} - p)} \quad (9)$$

421 where F_e is a model empirical constant and a_{nuc} is the nucleation-site volume fraction. These
 422 model constants have typical values of 50 and 0.0005, respectively, as suggested by Zwart et al.
 423 (2004) for the case of cavitation. R_b is an estimation of the mean-bubble diameter, which is in
 424 essence a model tuning parameter explicitly correlated to the nucleation-site density, as dictated
 425 by the formulation of the ZGB model. Besides, it must be noted that since, at flash boiling

432 conditions, no vapour condensation takes place, the phase-change term \dot{R} is activated when the
433 pressure-difference term in the square root of Eq. (9) becomes positive, while the same applies
434 for the respective terms of all models.

435 It is important to point out that the modelling approaches examined apart from the HRM
436 require the estimation of the density and distribution of activated nucleation sites for the
437 derivation of the mass-transfer rate. In fact, it has been verified that the mass-transfer rate
438 associated to flash boiling is significantly enhanced by the activation of additional nucleation
439 sites (Lamanna et al., 2014). In the cases examined in this study, it has been assumed that the
440 nucleation-site density is constant and equal to 10^{13} sites uniformly distributed per unit of the
441 liquid volume for the reasons that have already been reported in the discussion regarding the
442 derivation of **Eq. (2)**. In order to highlight the effect of the nucleation-site density on the
443 produced results, a correlation of the site-density N_b with the degree of superheat ΔT_{sup} proposed
444 by Senda and Hoyjo (1994) has also been considered, as follows:

$$445 \quad N_b = C_n \exp \left(\frac{-5.279}{\Delta T_{sup}} \right) \quad (10)$$

447 where C_n corresponds to the number of maximum available nucleation sites and is taken equal to
448 10^{13} .

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452

2.4 Homogeneous Equilibrium Model (HEM)

453 A numerical formulation of different principle, where a vapour fraction equation is not solved,
454 has also been considered in this study. The specific phase-change model is based on the
455 assumption of thermodynamic-equilibrium between the liquid/vapour phases, rendering the
456 mass-transfer rate at the bubble interface as infinite. Thus, an appropriate Equation of State
457 (EOS) directly linking pressure to density has been applied in order to describe the phase-change
458 process. The Tait EoS was employed for the liquid phase, while the vapour phase was assumed
459 an ideal gas. Referring to the mixture, the liquid/vapour phases were assumed to be in thermal
460 and mechanical equilibrium, while the pressure was taken to be equal to the saturation pressure
461 (Koop, 2008). The set of governing equations comprised the Navier-Stokes and energy
462 equations, solved for the homogenous fluid mixture of the liquid and vapour phases.

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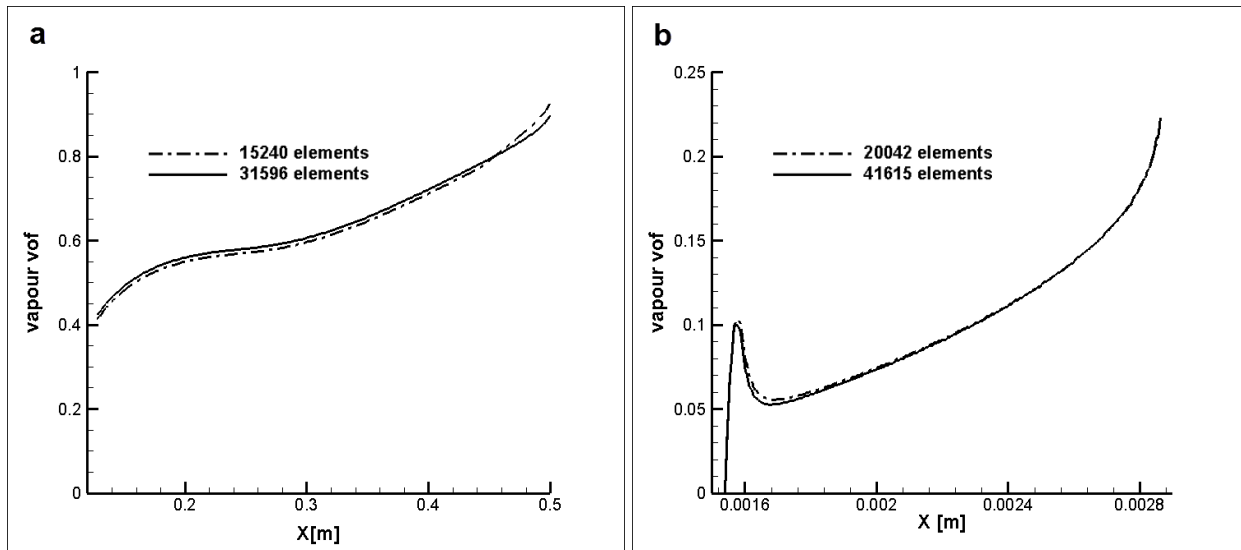
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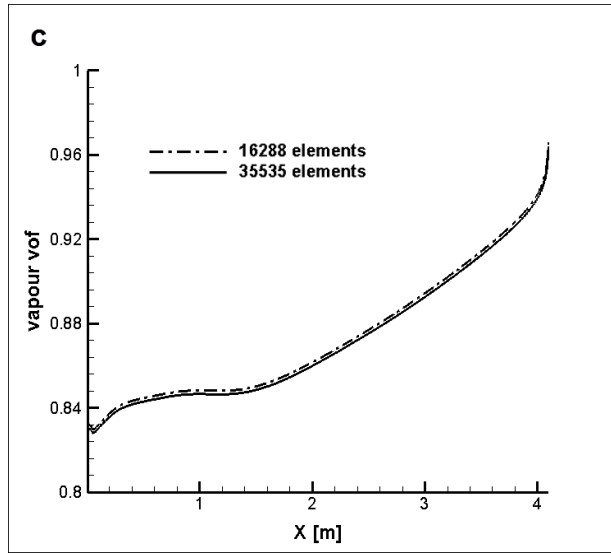
2.5. Grid-independence study

466 The sensitivity of the produced results to the grid resolution has been test for all the cases
467 examined by monitoring the effect of the grid density on the numerical results. The Hertz-
468 Knudsen model, **Eq. (3)**, was indicatively selected to model phase-change and consecutive tests
469 with computational grids of increasing density were performed for all cases. The grid topology in
470 reference to the three geometrical layouts can also be seen in **Fig. 1**. Vapour volume fraction
471 distributions were monitored at characteristic locations for each layout to judge on the grid
472 independence of the solution, since the phase-change rate influences the pressure, velocity and
473 temperature fields.

474 A total number of 15240, 20042 and 16288 grid cells were found to be sufficient for
 475 producing accurate results, in respect to the “Moby Dick”, “Reitz” and “Edwards” cases,
 476 respectively. Indicatively, referring to the regions of interest, in the “Moby Dick” case, the
 477 straight nozzle part was discretized with a cartesian grid of 28 (half cross-section) x 214 (length)
 478 cells. Likewise, the throttle region of the “Reitz” nozzle with a grid of 30 x 274 cells and the duct
 479 region of the “Edwards’ pipe” case by 8 x 819 cells, respectively. As shown in **Fig. 3**, further
 480 grid refinement had a negligible effect on the vapour fraction distribution for all cases. More
 481 specifically, the average vapour volume-fraction value at the wall of the straight nozzle section,
 482 as produced by a refined grid of 31596 elements for the Moby-Dick case (**Fig. 3a**), varied by
 483 0.6% compared to the respective value produced by a 15240-element grid. Refining the grid for
 484 the “Reitz” nozzle (**Fig. 3b**) from 20042 to 41615 elements resulted to a variation of less than
 485 0.7% in the average vapour fraction value at the throttle wall ($Y=0.00017$). Likewise, referring to
 486 the “Edwards’ pipe” case (**Fig. 3c**), a grid refinement from 16288 to 35535 elements lead to a
 487 discrepancy in the order of 0.2% in the average value of the vapour volume fraction at the duct
 488 wall ($X=0.038\text{m}$).
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Figure 3. Effect of the grid density on the vapour volume fraction distribution: (a) at the wall of the “Moby-Dick” nozzle straight section ($Y=0.01065\text{m}$), (b) at the throttle wall ($Y=0.00017\text{m}$) of the “Reitz” nozzle and (c) at the duct wall ($X=0.038\text{m}$) of the “Edwards’ pipe” for $t=0.3\text{s}$.

499 3. Results

500 The numerical results as produced employing **Eqs. (2)-(4), (7) and (9)** are presented in a
501 comparative manner in this section and validated against the available experimental data. The
502 flow field emerging in the “Moby Dick” nozzle is illustrated through the contour plots of the
503 pressure, velocity and temperature distributions in the throttle region ($0.4 < X < 0.64$) presented in
504 **Fig. 4**. The predictions of the two-phase model employing the Hertz-Knudsen **Eq. (3)** for a λ
505 value of 0.1 and the respective of HEM are indicatively shown in **Figs. 4a-f**, since, from a phase-
506 change rate perspective, they correspond to thermodynamic non-equilibrium and equilibrium
507 conditions, respectively. From a flow-topology point of view, it must be noted that the results
508 produced using the other two-phase models considered (Knudsen, HRM and ZGB) bear
509 resemblance to the ones shown in **Figs. 4a-c** referring to the Hertz-Knudsen model. The pressure
510 contours shown in **Figs. 4a** and **4d** illustrate a considerable flow depressurization occurring
511 downstream the nozzle throat. As can be also seen, the in-nozzle pressure values predicted by the
512 HEM are higher in comparison to those produced by the Hertz-Knudsen model. This trend is
513 attributed to the effect of the phase-change rate on the pressure distribution, as will be explained
514 in more detail in the next paragraph referring to the Reitz case. The insets of **Figs. 4a** and **4d**
515 elucidate that the pressure distribution obtains a minimal value at a location further downstream
516 the nozzle throat, before adjusting to higher pressures, i.e. a shockwave is formed. Contours of
517 the pressure-gradient magnitude are also depicted as black lines on the insets, in order to
518 illustrate the formation of the shockwave, since, the gradient obtains large values at the location
519 of formation. Both models predict the shockwave, however at non-coincident locations, since
520 according to the HEM prediction, the shockwave forms approximately at $X=0.82\text{m}$, instead of
521 $X=0.67\text{m}$ as predicted by the Hertz-Knudsen model. **Figs 4b** and **4e**, depicting the velocity
522 distribution, also reveal that the flow is accelerated at the divergent region, a clear indication of
523 the expansion of initially under-expanded two-phase flow, which is associated with the

524 formation of a shockwave (Prudhomme and Haj-Hariri, 1994). The maximum velocity predicted
 525 by the HEM (**Fig. 4e**) in the expanding nozzle part is significantly higher than the respective of
 526 the two-phase, Hertz-Knudsen model (**Fig. 4b**), owing to the higher in-nozzle pressure predicted
 527 for equilibrium conditions, which leads to a more severe flow expansion downstream the nozzle
 528 throat. The Mach number distributions also depicted in **Figs. 4b** and **4d**, were calculated as the
 529 fraction of the mixture velocity to the respective local sonic velocity c , i.e. $M=u/c$. In the case of
 530 the HEM, where phase change is instantaneous and described through an EoS, the local sonic
 531 velocity is derived directly from the definition, i.e. $c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$, e.g. see Koop (2008):

532

$$533 \frac{1}{c_{mix}^2} = \frac{c_{v,mix}}{c_{p,mix}} \left(\frac{\partial \rho_{mix}}{\partial p} \right)_T \quad (11)$$

534

535 where $c_{v,mix}$ and $c_{p,mix}$ correspond to the specific heat at constant volume and pressure,
 536 respectively. For two-phase models, where, in concept, the mass-transfer rate is not “infinite”,
 537 the following correlation, as suggested by Franc and Michel (2005) is implemented in Fluent
 538 (ANSYS FLUENT, 2012):

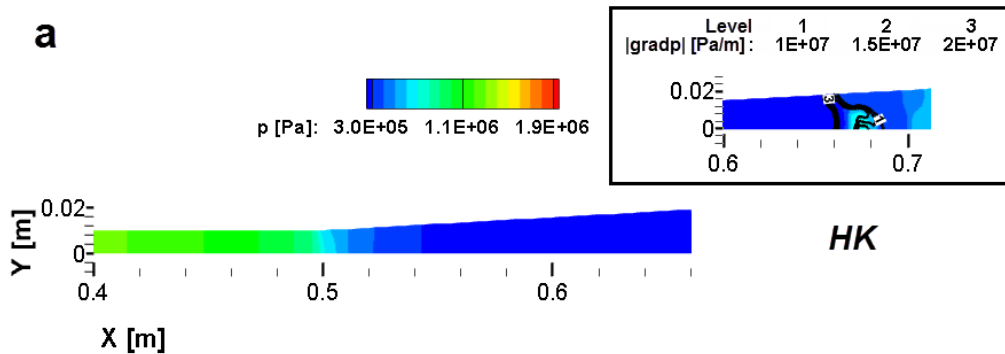
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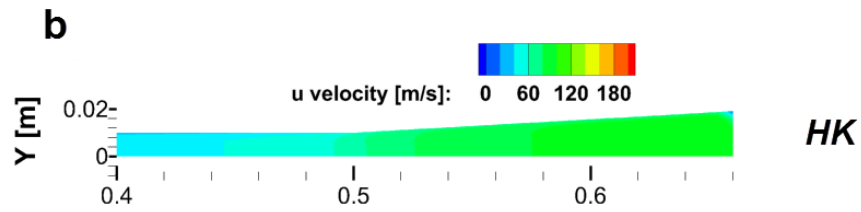
$$540 \frac{1}{\rho_{mix} c_{mix}^2} = \frac{a_v}{\rho_v c_v^2} + \frac{1-a_v}{\rho_l c_l^2} - \frac{\dot{R}}{\rho_v dp} \quad (12)$$

541

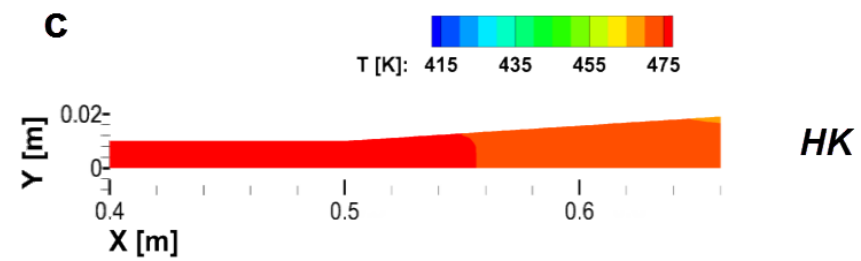
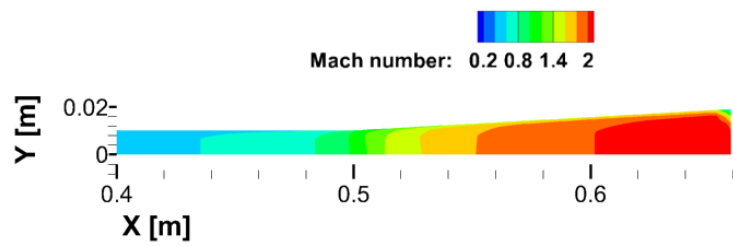
542 where c_l and c_v are the respective sonic velocities for the liquid and vapour phases, while the
 543 third term on the right hand side of the equation corresponds to the effect of phase-change on the
 544 mixture compressibility. As illustrated by the plots, the flow obtains sonic velocity ($M=1$) in the
 545 vicinity of the nozzle throat and further accelerates, thus becoming supersonic, at the divergent
 546 nozzle part. It must be noted that the sonic velocity that, in essence adjusts the flow velocity is
 547 different depending on the phase-change modelling approach, as it is designated by the local
 548 phase-field distribution. **Figs. 4c** and **4f** depicting the temperature field emerging at the throttle
 549 region and downstream verify this deduction, since the jet cooling predicted by the HEM is much
 550 more pronounced compared to the Hertz-Knudsen model, i.e. approximately 60K instead of 10K.
 551 The mixture temperature decreases due to the latent heat exchange required for bubble
 552 nucleation.

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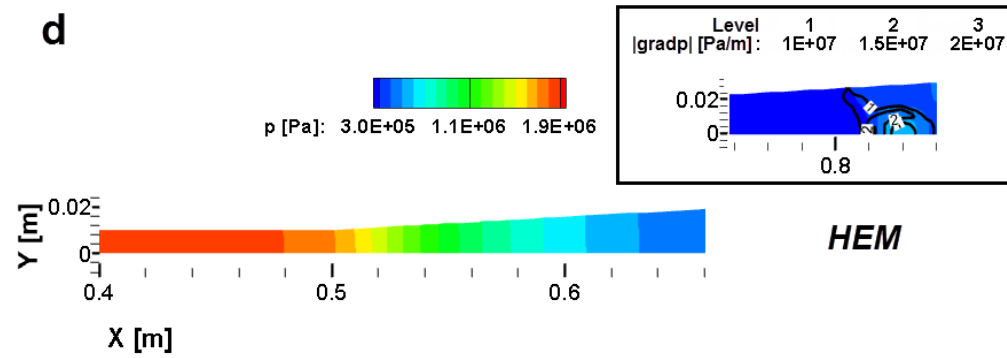




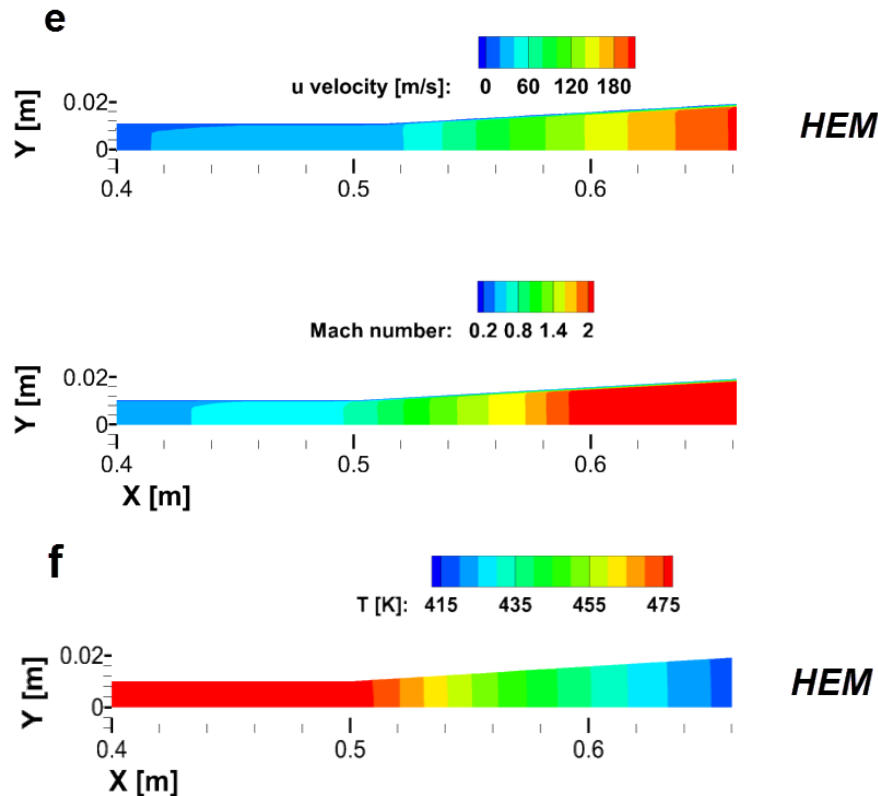
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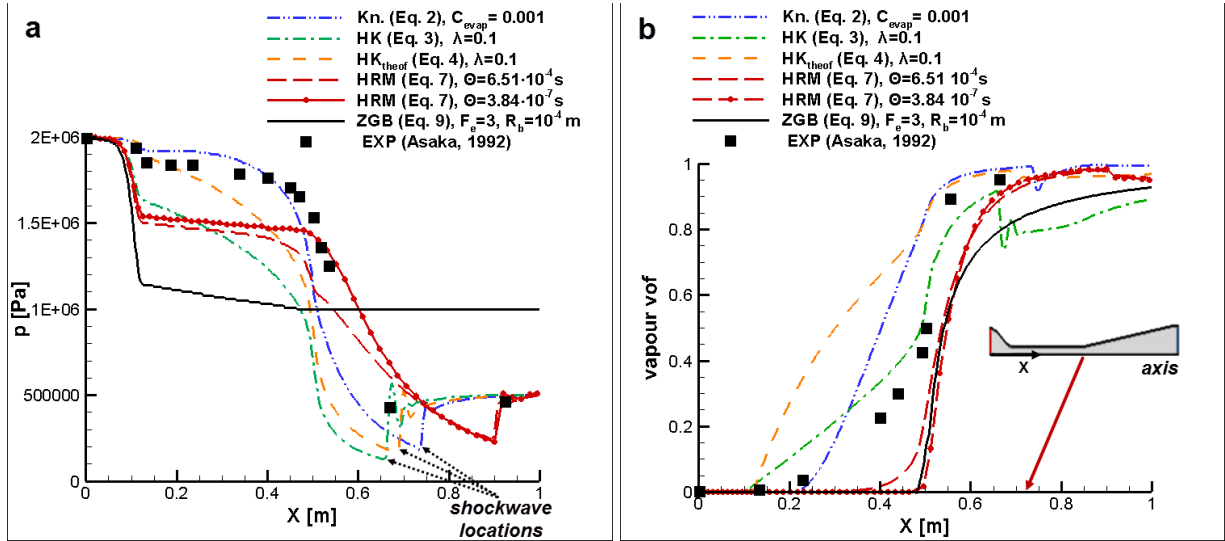
560 **Figure 4.** “Moby Dick” nozzle-Contour plots of (a, d) the pressure, (b, e) velocity and (c, f)
 561 temperature fields at the throttle region, as predicted using Hertz-Knudsen Eq. (3) for $\lambda=0.1$ (a-c)
 562 and HEM (d-f).

563

564 **Fig. 5** depicts the pressure (**Fig. 5a**) and vapour volume fraction (**Fig. 5b**) distributions at the
 565 nozzle main axis. The comparison between the numerical predictions and the available
 566 experimental data of Asaka (1992) in reference to the pressure distribution illustrates that the
 567 models based on the kinetic theory of gases predict a more gradual liquid depressurization,
 568 compared to the HRM model with the closest agreement being accomplished for the predictions
 569 of the Knudsen model (**Eq. 2**). Referring to HRM, the pressure distribution produced using the
 570 “high-pressure” formulation exhibits higher values in the nozzle convergent part, which are in
 571 better matching with the experimental points, as expected since the inlet pressure is higher than
 572 10 bar, compared to the predictions of the respective “low pressure” format. The discontinuity in
 573 the distribution observed at the divergent nozzle part ($X>0.65$) is associated with the shockwave
 574 formation due to flow expansion, as also illustrated in **Fig. 4a**. The ZGB model seems to be
 575 failing to predict both qualitatively and quantitatively the pressure drop within the nozzle, as the
 576 steep reduction predicted shows significant discrepancy to the experimental data.

577 The respective plot for the vapour volume fraction distribution (**Fig. 5b**) illustrates that almost
 578 full liquid vaporization has occurred at an axial distance of 0.65m. Adequate agreement exists
 579 between the predictions of all models and the experimental data. In fact, the closest matching to
 580 the experimental points is achieved by the predictions of the Hertz-Knudsen **Eq. (3)** for a value
 581 of the accommodation coefficient λ of 0.1, which suggests significant deviation from
 582 thermodynamic equilibrium. At this point, it must be highlighted that the ZGB model has been

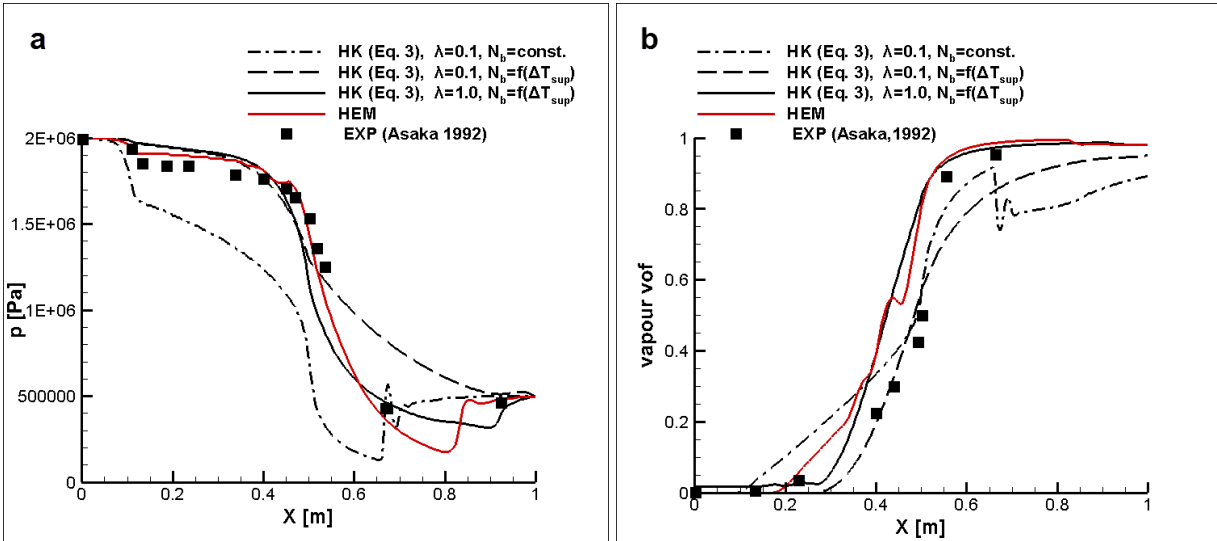
583 significantly tuned, as the suggested value of 50 (Zwart et al., 2004) for the calibration
 584 coefficient F_e (see **Eq. 9**) produced a very steep phase-change process, highly deviating from the
 585 experimental data with almost full vaporization of the liquid at a location close to $X=0.35$. A
 586 sensitivity analysis was performed and a value of $F_e=3$ was eventually set, as it was found to
 587 produce results of acceptable agreement with the experimental data in reference to the vapour
 588 volume fraction distribution. This value ($F_e=3$) has been employed for all the test cases
 589 presented in this study. However, the model calibration (for $n_b=10^{13} \text{ m}^{-3}$) did not produce
 590 satisfactory results regarding the pressure distribution and further examination of the influence of
 591 the additional model coefficients (a_{nuc} and R_b), associated with the nucleation-site distribution,
 592 on the overall phase-change rate was deemed not to be within the scope of the present study.
 593 The specific model is oriented to cavitating flows and has been included in this investigation
 594 only as a reference, in order to confirm that, despite the similar macroscopic manifestation of the
 595 two phenomena, caution should be taken on the mechanism adopted for the modelling of the
 596 actual phase-change process.
 597



598
 599
 600 **Figure 5.** “Moby Dick” nozzle-Comparison of the numerical predictions to available
 601 experimental data: (a) Pressure and (b) vapour volume fraction at the axis along the nozzle
 602 length.
 603

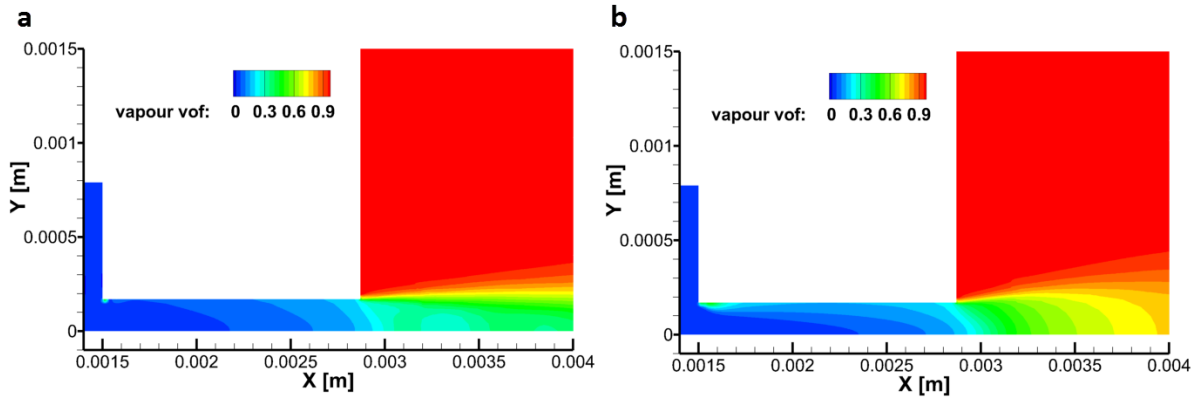
604 It must be pointed out that the predictions presented so far were produced considering a
 605 constant number of 10^{13} nucleation sites per unit volume. The effect of the nucleation-site
 606 density N_b on the numerical results is illustrated by **Fig. 6**, which depicts the predictions of the
 607 Hertz-Knudsen model (**Eq. 3**) for the “Moby Dick” case considering both constant and variable
 608 distributions of the nucleation-site density. In the latter case the distribution is correlated to the
 609 liquid superheat through **Eq. (10)**. The predictions based on a constant distribution of nucleation
 610 sites correspond to the dash-dot line of **Fig. 5** and have been added to **Fig. 6** as reference values.
 611 It can be clearly discerned in **Fig. 6a** that the pressure distribution predicted for $\lambda=1$, which
 612 corresponds to conditions close to thermodynamic equilibrium, and variable N_b exhibits an
 613 excellent agreement with the experimental data, while the respective distribution for $\lambda=0.1$
 614 corresponds to a much more gradual pressure decrease at the throttle region. Likewise, as

615 depicted in **Fig. 6b**, the distribution of the vapour volume fraction for $\lambda=1.0$ and variable N_b ,
 616 exhibits a very good match to the experimental data. The numerical predictions for the same
 617 case, as produced the HEM model are also depicted in **Fig. 6**. It is evident that the predictions of
 618 the equilibrium model, in which there are no considerations on nucleation sites but rather
 619 appropriate EoS are used, are in agreement with the respective of the Hertz-Knudsen model for
 620 $\lambda=1$. Hence, it can be deduced that the phase-change rate in the “Moby Dick” case is plausible to
 621 be corresponding to thermodynamic equilibrium. However, at this point it must be commented
 622 that the effects of these intrinsic two-phase flow features, i.e. activated nucleation-site
 623 distribution and prevailing thermodynamic conditions, are not distinguishable in a
 624 straightforward manner, since both lead to the augmentation of the overall phase change rate.
 625



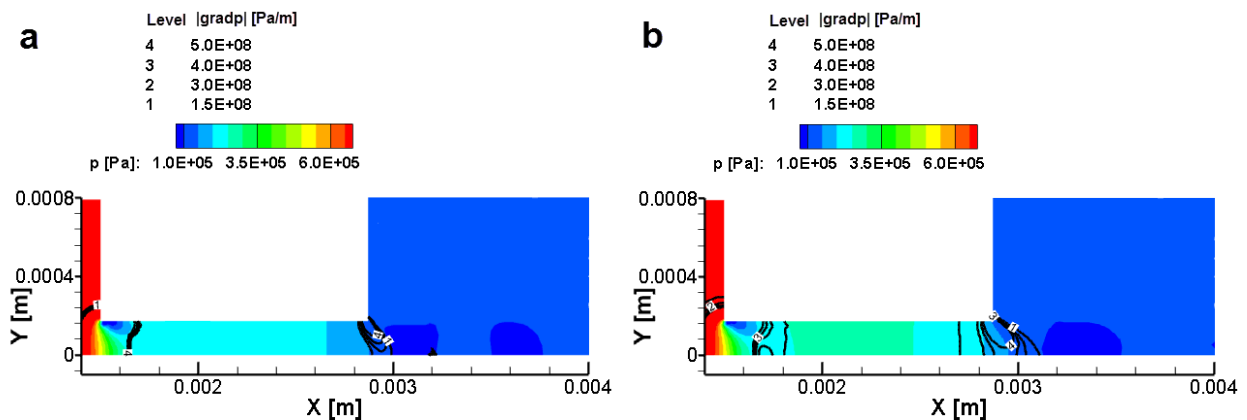
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 628 **Figure 6.** “Moby Dick” nozzle-Effect of the nucleation-site density distribution on the produced
 629 results: (a) pressure and (b) vapour volume fraction distribution.
 630

631 Referring to the “Reitz” benchmark configuration, predictions of the phase field emerging
 632 within the nozzle are presented in **Fig. 7**. It can be clearly discerned that the bubble nucleation
 633 commences at the throttle vertex and gradually expands from the nozzle wall to the orifice axis.
 634 The low pressure at the throttle entrance due to flow separation at that region acts as the
 635 necessary perturbation for phase change to commence. Less extensive mass-transfer rate
 636 throughout the fluid bulk is predicted by the Hertz-Knudsen model, **Eq. (3)**, (**Fig. 7a**) compared
 637 to the HRM (**Fig. 7b**). The predictions of both models are in agreement with the qualitative
 638 findings of Reitz (1990), who reported that the liquid core could be discerned at the nozzle outlet
 639 and that severe atomization sets in immediately downstream the nozzle outlet. This “liquid core”
 640 is more pronounced in the predictions of the Hertz-Knudsen model, which in general predicts
 641 lower vapour volume-fraction values slightly downstream of the nozzle outlet compared to the
 642 HRM.



643
 644 **Figure 7.** “Reitz” nozzle-Contour plots of the phase field for $T=427\text{K}$: (a) Hertz-Knudsen, Eq.
 645 (3) ($\lambda=0.1$), (b) HRM, Eq. (7) ($\Theta=6.51 \cdot 10^{-4}\text{s}$).
 646

647 The pressure field in the “Reitz” nozzle as produced indicatively by the Hertz-Knudsen **Eq.**
 648 (3) and HRM, **Eq. (7)**, models is depicted in **Fig. 8**. As illustrated by both plots, a low pressure
 649 region sets in at the throttle entrance due to the flow separation. Further downstream, the flow
 650 retains relatively constant pressure values, while it drops to its atmospheric value in the vicinity
 651 of the nozzle outlet. The HRM model (**Fig. 8b**), in general, predicts higher pressure values in the
 652 largest part of the throttle compared to the Hertz-Knudsen model (**Fig. 8a**). As illustrated by the
 653 comparative plot of **Fig. 8c**, according to HRM results, pressure values are approximately 25%
 654 higher compared to the respective predictions based on the the Hertz-Knudsen model in a
 655 significant part of the throttle ($0.0018 < X < 0.0025$). This trend is associated with the higher
 656 mass-transfer rate predicted by the specific model (see **Fig. 7**), which, in turn, has a more
 657 considerable impact on the mixture compressibility in the nozzle region (Franc and Michel,
 658 2005). The flow expansion downstream the injector outlet is associated with the formation of
 659 shockwaves, predicted by both models; the shockwave locations are signified by the low
 660 pressure regions downstream the outlet, as well as by the contours of the pressure-gradient
 661 magnitude, also plotted in **Figs. 8a-b** as black lines, which illustrate that significant flow
 662 depressurization occurs in the near-nozzle region. Further downstream, the pressure re-adjusts to
 663 the atmospheric value.
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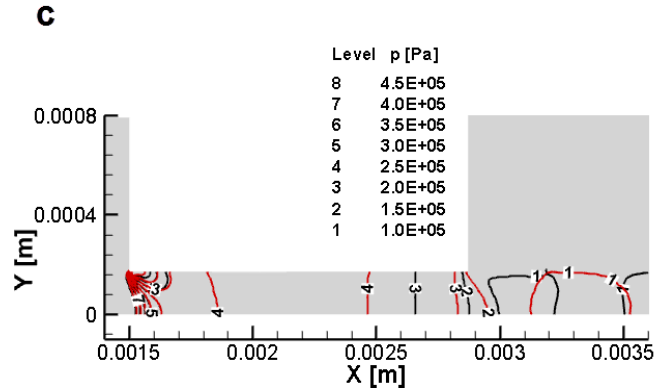
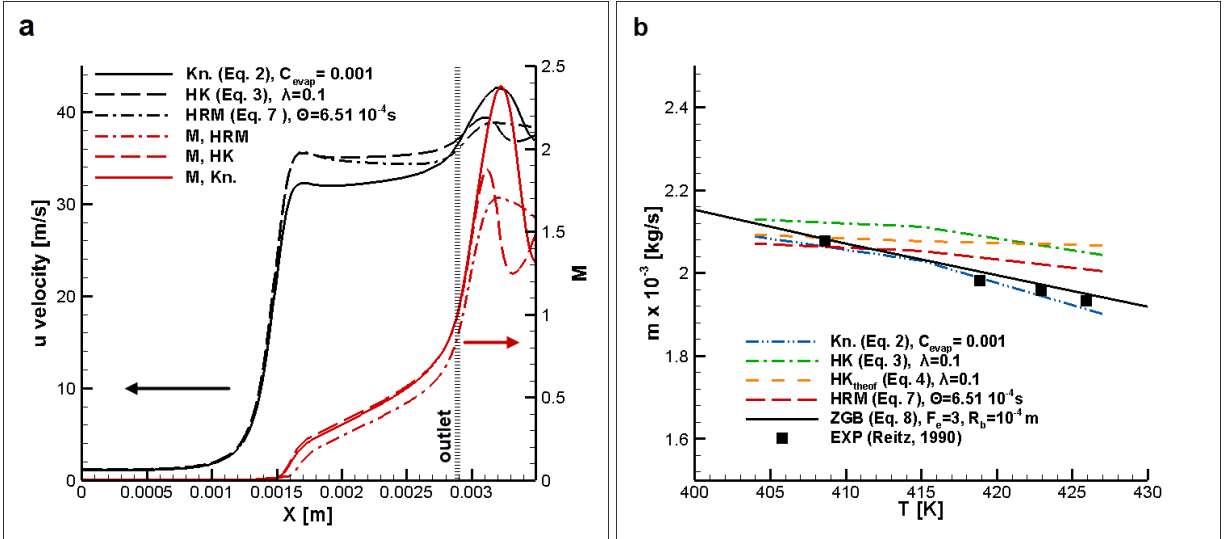


Figure 8. “Reitz” nozzle-Contour plots of the pressure field for $T=427\text{K}$: (a) Hertz-Knudsen, Eq. (3) ($\lambda=0.1$), (b) HRM, Eq. (7) ($\Theta=6.51 \cdot 10^{-4}\text{s}$) and (c) comparative contour plot with black and red lines corresponding to the predictions of HK and HRM, respectively.

Fig. 9a depicts the axial velocity distribution along the “Reitz” nozzle axis. It is evident that the flow is significantly accelerated as it enters the throttle region, where it subsequently retains relatively constant values. The Mach number ($M=u/c$) distribution for the two-phase mixture is also plotted on **Fig. 9a** and it illustrates that the flow velocity becomes equal to the speed-of-sound velocity c ($M=1$) at the outlet region, i.e. choked-flow conditions are reached. Downstream the outlet, the expansion of the two-phase mixture constitutes the flow supersonic, with the predicted Mach numbers being in the range 1.7-2.4. The predictions of the three models depicted in **Fig. 9a** have a similar form with the Knudsen mass-transfer model predicting a slightly higher acceleration downstream of the nozzle outlet.

The effect of the liquid temperature on the mass flow rate through the nozzle inlet is depicted in **Fig. 9b**. As can be seen, the flow rate is decreased by approximately 10% in the temperature range considered 400-427K as the extent of the nozzle cross-sectional area occupied by vapour increases due to the increased phase-change rate and thus the available active area for the liquid to flow decreases. The predictions of all models are in good agreement with the experimental data available by Reitz (1990) and the minor flow-rate decrease is well captured by all models. The calibrated ZGB model in the specific case seems capable of capturing a macroscopic flow features, such as the overall mass-flow rate. Besides, it must be noted that numerical results shown in **Fig. 9b** correspond to low-phase change rate indicative of non-equilibrium conditions (Koukouvinis et al., 2016). A parametric study was conducted, so as to further verify that the thermodynamic conditions in reference to the “Reitz” case correspond to non-equilibrium. The case for $T=427\text{K}$ was considered and the numerical predictions produced by the Hertz-Knudsen model, Eq. (3), for different combinations of λ and n_0 were compared against the experimental value for the inlet mass flow rate. As can be deduced from the values of **Table 1**, the closest agreement to the experiment is accomplished for the set of parameters selected for the production of the results presented in **Figs. 7-9**, i.e. $n_0=10^{13}$ and $\lambda=0.1$. Increasing the λ value to 1 leads to the prediction of significantly lower mass-flow rate due to the enhanced in-nozzle phase-change rate, while the discrepancy from the experimental value is increased. This signifies that the flow conditions in the “Reitz case” are characterized by a strong deviation from thermodynamic equilibrium.



701
 702 **Figure 9.** “Reitz” nozzle: (a) Velocity and Mach number distributions at the nozzle axis and (b)
 703 mass-flow rate at the nozzle inlet.

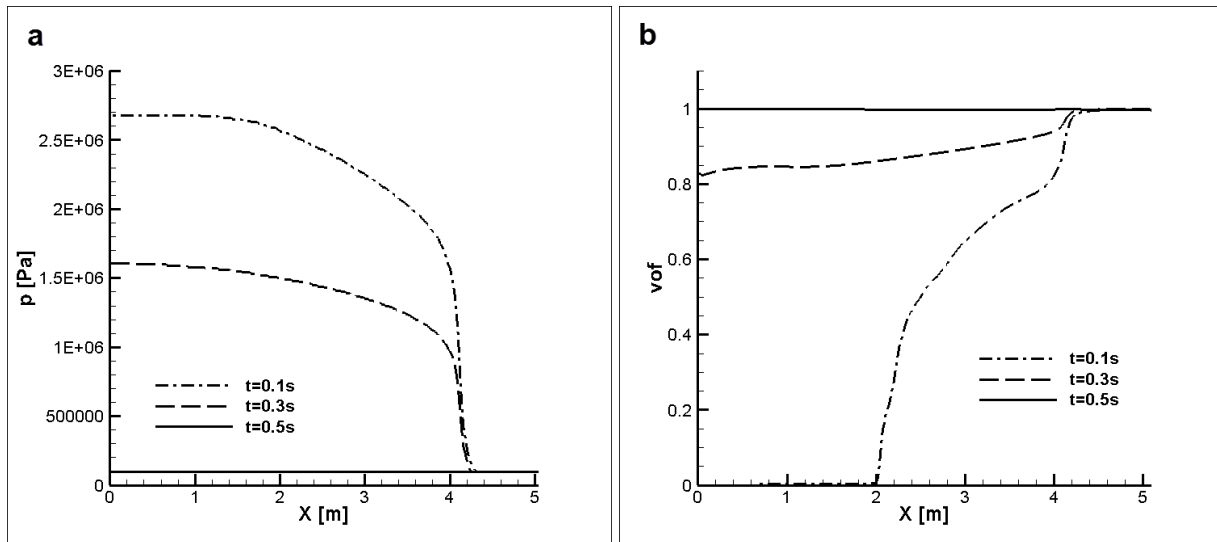
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Table 1. Predictions of the Hertz-Knudsen model for different λ and n_0 values.

λ	n_0 [m ⁻³]	\dot{m} [g/s]	Deviation (%)
0.1	const. (=10 ¹³)	2.043	5.68
1.0	const. (=10 ¹³)	1.662	14.02
0.1	$f(\Delta T_{sup})$ Eq. (10)	2.097	8.50
1.0	$f(\Delta T_{sup})$ Eq. (10)	1.747	9.60

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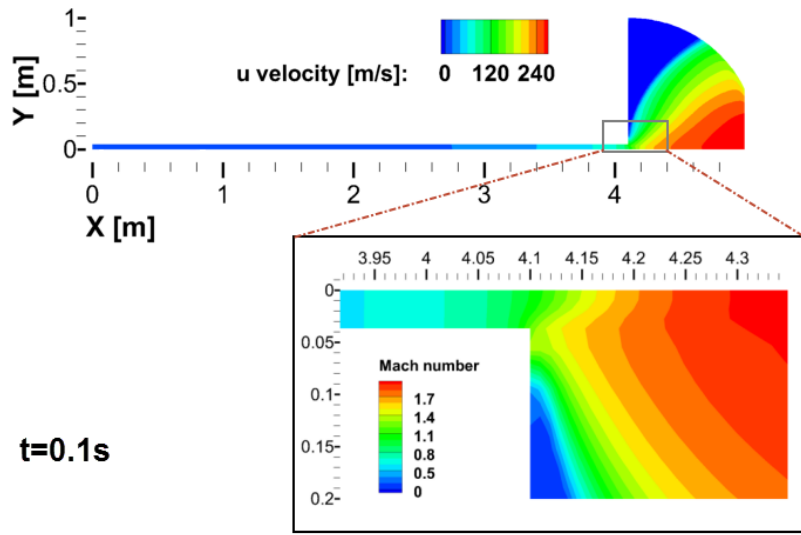
The pressure and vapour volume fraction distributions at the axis of the “Edwards’ pipe”, the third benchmark geometry examined in this study, are depicted for different time instances in **Fig. 10**. As made evident by **Fig. 10a**, a rarefaction wave propagates with the speed of sound of the liquid phase into the pipe. The pressure continues to drop, until atmospheric conditions prevail throughout its entire volume at approximately 0.5s. **Fig. 10b** illustrates that phase change commences exactly at the pipe outlet and the vaporization front travels upstream towards the inlet, as indicated by the line corresponding to $t=0.1$ s. Almost full liquid vaporization has occurred after 0.5s from the beginning of the transient flow process.



716
 717 **Figure 10.** Edwards' (a) Pressure and (b) vapour volume fraction distributions at the duct axis
 718 for various time instances (Hertz-Knudsen Eq. (3), $\lambda=0.1$): (a) $t=0.1$ s, (b) $t=0.3$ s and (c) $t=0.4$ s.
 719

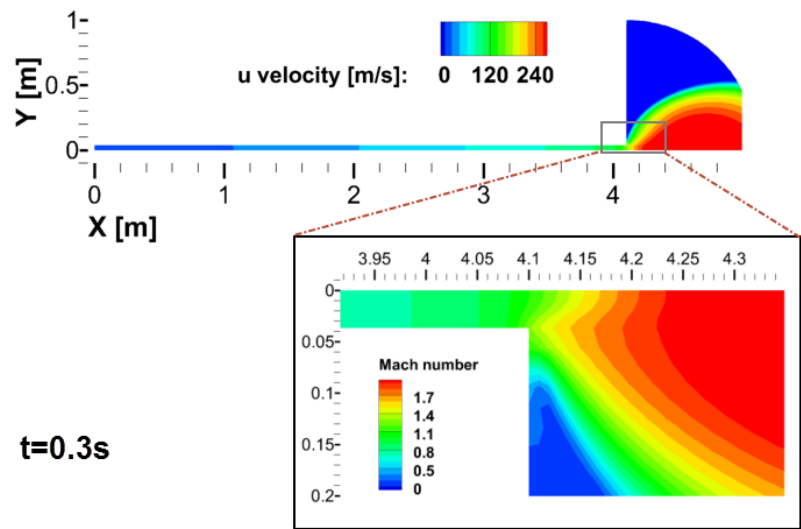
720 The temporal evolution of the velocity field is illustrated by the contour plots of **Fig. 11**. As
 721 can be seen, the flow is significantly accelerated towards the pipe outlet and the two-phase jet is
 722 expelled to ambient with an increased cone angle. The increased cone angle is once again due to
 723 the expansion of the mixture fluid downstream the nozzle outlet. The detailed view of the Mach
 724 number distribution in the vicinity of the duct outlet, also depicted in **Fig. 11**, confirms that the
 725 flow is choked (Mach number equal to unity) for all time instances shown and that the two-phase
 726 mixture expands to supersonic flow further downstream. As the phenomenon evolves and hence
 727 the vaporization front reaches closer to the pipe left end, the local velocity in the vicinity of the
 728 outlet, which is adjusted by the local phase field, increases from approximately 80m/s at $t=0.1$ s
 729 (**Fig. 11a**) to 180m/s at $t=0.4$ (**Fig. 11c**), while at the same time the downstream region of
 730 elevated velocities is reduced. It must be highlighted that the flow remains choked even for
 731 $t=0.4$ s, however the downstream expansion is less pronounced compared, e.g., to $t=0.1$ s. Hence,
 732 it is logical to deduce that as the local mixture quality at the outlet approaches pure vapour, the
 733 local speed-of-sound velocity, which adjusts the flow velocity in the duct, increases and
 734 consequently the flow expansion becomes less violent.
 735

a

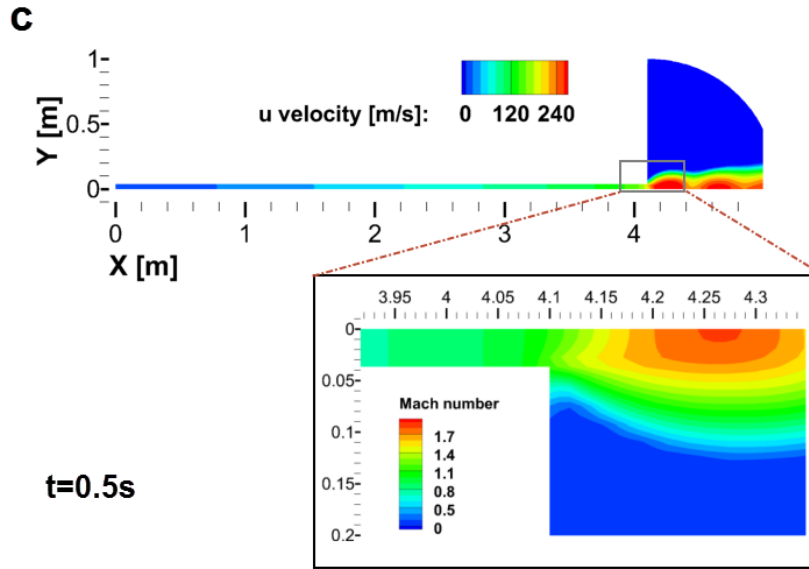


736

b



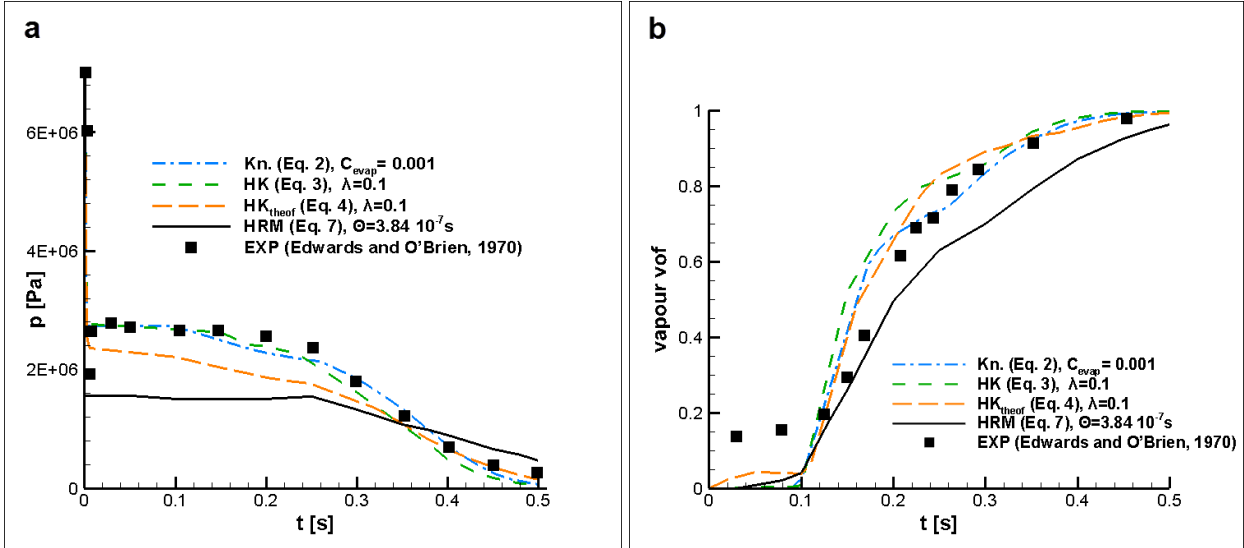
737



738
 739 **Figure 11.** “Edwards’ pipe”-Contour plots depicting time instances of the velocity field (Hertz-
 740 Knudsen Eq. 3, $\lambda=0.1$): t=0.1s, (b) t=0.3s and (c) t=0.4s.

741
 742 **Fig. 12** depicts the comparison between the predictions of four two-phase models, namely
 743 **Eqs. (2)-(4)** and (7) and the experimental data available by Edwards and O’Brien (1970)
 744 regarding the time evolution of the pressure at the pipe head and the vapour volume fraction at
 745 the pipe mid-section. It was decided the ZGB not to be tested in the present case, since its
 746 formulation has not been suggested for cases where mass-transfer occurs through a single
 747 interphase, as in the “Edwards’ pipe” case. As can be seen the Knudsen and Hertz-Knudsen
 748 **Eqs. (2)-(4)** considering a λ value of 0.1 produce accurate predictions regarding both pressure
 749 (**Fig. 12a**) and vapour volume fraction (**Fig. 12b**). Specifically referring to the volume fraction
 750 distribution, it has to be commented that, as can be seen on **Fig. 12b**, the first two experimental
 751 points cannot be captured by the Hertz-Knudsen models. However, failure of the models to
 752 accurately capture the phase field should also reflect to their predictions regarding the pressure
 753 field, since the mass-transfer rate affects the mixture compressibility, as has been pointed out in
 754 the previous paragraphs. Yet the predictions are in agreement to the experimental data with
 755 regard to pressure. Furthermore, the working medium has not been characterized in terms of gas
 756 content or impurities and the experimental uncertainties associated with the data have not been
 757 reported and thus the possibility of non-condensable gas effects to be responsible for the
 758 discrepancy detected cannot be assessed. Gas bubbles serving as nucleation sites should be
 759 expected to enhance the vaporization rate throughout the evolution of the phenomenon and hence
 760 the discrepancy between experimental data and numerical prediction should ensue for all time
 761 instances. For low vapour-fraction values in the order of 15%, more plausible explanations for
 762 the deviation are considered the relatively high experimental error associated with such values,
 763 which correspond to low signal to noise ratio for the measuring sensor, or possible density
 764 fluctuations that are recorded as vapour generation (see Mauger et al., 2012). Hence, the
 765 predictions validity of the models based on the kinetic theory of gases regarding flashing flows
 766 can be considered to have been verified for all the flow configurations examined in the present
 767 investigation.

768 The “high pressure” formulation of the HRM was deemed as suitable for predicting the flow
 769 in the “Edwards pipe” case, in which the initial pressure substantially exceeds 20 bar. The
 770 respective results, also depicted on **Fig. 12** demonstrate that the flow can be qualitatively
 771 captured in terms of both the pressure and vapour volume fraction distribution, however a more
 772 significant depressurization is predicted by the model compared to the experimental data (**Fig.**
 773 **12a**) and this is attributed to the lower mass-transfer rate predicted (**Fig. 12b**), as has been
 774 already discussed in the previous paragraphs of this section. The quantitative deviation between
 775 the HRM predictions and the experiment is probable to stem from the semi-empirical parameters
 776 associated with the model, since their values have been determined considering steady, inlet-
 777 outlet flows with distinct differences from this case.
 778



779
 780 **Figure 12.** “Edwards’ pipe”-Comparison of the numerical predictions to experimental data: (a)
 781 pressure at the pipe (left) outer wall, (b) vapour volume fraction at the pipe mid-section.
 782

783 **4. Conclusions**

784 Different two-phase, mass-transfer models based on fundamental concepts such as the kinetic
 785 theory of gases, thermodynamic non-equilibrium and bubble-dynamics considerations, as well as
 786 a homogeneous equilibrium model, have been evaluated in a comparative manner in the present
 787 numerical investigation. The models based on the kinetic theory of gases, were found to produce
 788 accurate predictions regarding all the benchmark geometries considered, while the HRM model
 789 was also capable of capturing the two-phase flow in all cases, yet producing results with higher
 790 discrepancy to the experiment compared to Knudsen and Hertz-Knudsen mechanisms. On the
 791 contrary, the applicability of ZGB model was demonstrated to be doubtful. Especially regarding
 792 the ZGB model, which has been formulated for the prediction of cavitating flows, the phase-
 793 change rate that results if the standard model coefficient values are used is much higher than the
 794 one indicated by the experimental data. Therefore, although the two phenomena, i.e. cavitation
 795 and flash boiling macroscopically may seem as similar, it has been confirmed that the underlying
 796 phase-change mechanisms are of different nature.

797 The numerical results were demonstrated to be highly sensitive to the distribution of the
798 activated nucleation sites, which has a significant influence on the overall phase-change process
799 and its accurate determination is a prerequisite conditions prior to making any deductions in
800 reference to the deviation of the flashing flow from thermodynamic-equilibrium conditions.
801 Besides, the effects of the bubble-growth mechanism and the nucleation-site density on the
802 overall phase change rate cannot be distinguished, since they both act in an enhanceive manner.
803 Referring to the flow phenomena associated with the onset of flash boiling conditions, it was
804 verified through the numerical predictions that the phase and velocity fields are strongly linked,
805 as the local speed-of-sound velocity is designated by the quality of the liquid/vapour mixture
806 and, in turn, limits the local flow velocity. Flow choking due to effect of phase change takes
807 place at the location of the geometrical constriction followed by expansion in the diverging part
808 of the geometry, increase of the jet cone angle and formation of shockwaves in the vicinity of the
809 outlet region. Flow expansion has been found to be linked to enhanced spray atomization and
810 therefore the next step of future research will be to utilize the validated models in simulations of
811 realistic fuel injector configurations.

812
813

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