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Accuracy of Eulerian – Eulerian, two-fluid CFD boiling models of subcooled boiling flows

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ABSTRACT

Boiling flows are frequently found in industry and engineering due to the large amount of heat that can be transferred within such flows with minimum temperature differences. In the nuclear industry, boiling affects in different ways the operation of almost all water-cooled nuclear reactors. Recently, the use of Computational fluid dynamic (CFD) approaches to predict boiling flows is increasing and, in the nuclear area, CFD is being developed to solve thermal hydraulic safety issues such as establishing the critical heat flux, which is perhaps the major threat to the integrity of nuclear fuel rods. In this paper, the accuracy of an Eulerian – Eulerian, two-fluid CFD model is evaluated over a large database of subcooled boiling flows, avoiding the rather popular case-by-case tuning of descriptive models to a limited number of experiments. The model includes a Reynolds stress turbulence model, the method of moments-based S_γ population balance approach and a boiling model derived using the heat flux partitioning approach. The database covers a large range of conditions in subcooled boiling flows of water and refrigerants in vertical pipes and annular channels. Overall, a satisfactory predictive accuracy is achieved for some quantities of interest, such as the void fraction and the turbulence and liquid temperature fields, but results are less satisfactory in other areas, more specifically for the average bubble diameter and the mean velocity profiles close to the wall in annular channels. Agreement may be improved with advances in the treatment of large bubbles and bubble break-up and coalescence, as well as in improved modelling of the boiling region close to the wall, and more specifically the bubble departure diameter, the wall treatment and the contribution of bubbles to turbulence.

KEYWORDS: Subcooled boiling; computational fluid dynamics; two-fluid model; heat-flux partitioning; boiling model.

40 **1 Introduction**

41

42 In industry, boiling flows are often encountered because of the efficiency of heat transfer
43 mechanisms under such conditions, which allow the transfer of significant amounts of heat
44 with a limited amount of wall superheat, to the benefit of many engineering processes. In the
45 nuclear industry, different types of boiling regimes are found in all water-cooled reactors,
46 both in normal operation and during design-basis and beyond design-basis postulated
47 accident transients. Boiling water reactors operate in the saturated boiling regime, and some
48 degree of subcooled boiling is always experienced in pressurized water reactors during
49 normal operation. Buoyancy-driven natural circulation loops and safety systems are also
50 sometimes designed to operate within the boiling regime and, during loss of coolant accidents
51 for example, boiling may occur due to the decrease in pressure and the reduced coolant
52 inventory. For a reactor experiencing boiling conditions, the maximum amount of heat
53 transferrable from the nuclear fuel to the coolant is referred to as the critical heat flux (CHF)
54 and, when this is reached, the heat transfer deteriorates rapidly [1,2]. Recently, a significant
55 portion of nuclear reactor thermal hydraulic analyses make use of multiphase computational
56 fluid dynamic (CFD) models, and in particular of the Eulerian-Eulerian, averaged two-fluid
57 formulation that is invariably used when addressing industrial-scale engineering problems.
58 With respect to the simplistic models more commonly used in the nuclear industry, CFD may
59 ultimately be able to describe phenomena in much greater detail, leading to the solution of
60 selected nuclear reactor thermal hydraulic safety issues [3], including the prediction of CHF
61 which, despite being perhaps the main threat to the integrity of nuclear fuel rods and despite
62 long-term research efforts, has still resisted accurate modelling and understanding [4].

63 With the aim of predicting the boiling process, different wall boiling models have been
64 incorporated in modern CFD codes. For two-fluid averaged models, these approaches are in
65 the large majority based on the Rensselaer Polytechnic Institute (RPI) boiling model from
66 Kurul and Podowski [5], where the heat flux from the wall is partitioned between the
67 mechanisms responsible for the heat transfer process, these being single-phase convection,
68 quenching and evaporation. In recent years, many authors have used more or less refined
69 versions of the RPI boiling model to predict boiling flows [6-12]. After departure from the
70 heated wall, the bubbles join the bulk of the flow and the size distribution of these bubbles,
71 polydispersed in general, governs interphase exchanges of mass, momentum and energy.
72 Therefore, in models of these flows, knowledge of the average diameter of the bubbles is
73 required in many closure relations, and additional models have been used to predict the

74 average bubble diameter distribution. Initially, bubble size was derived from experimental
75 data or empirical correlations of subcooling in the liquid phase [5,13-16]. More recently,
76 bubble size distribution has been predicted by coupling different population balance
77 approaches to the two-fluid and the wall boiling models. Yao and Morel [6] derived source
78 terms for bubble coalescence, bubble break-up and phase change to be used in the volumetric
79 interfacial area transport equation. Yeoh and Tu [7] added wall nucleation and condensation
80 in the bulk flow to the multiple size group (MUSIG) model [17], which divides the bubble
81 diameter spectrum into a finite number of ranges to accommodate non-uniform bubble size
82 distributions. All these authors reported significant improvements over predictions based on
83 empirical correlations of subcooling of the liquid phase. More recently, Krepper et al. [10]
84 applied the inhomogeneous version of the MUSIG model, where each bubble size range is
85 allowed to have its own velocity, to the simulation of a subcooled boiling flow in a vertical
86 pipe. Morel and Lavieville [18] extended to boiling flows a method based on conservation of
87 the density S_γ of the moments of the bubble size distribution, which was assumed to obey to a
88 log-normal probability distribution. In their model, bubble break-up was not accounted for.
89 Bubble break-up was considered in the context of the S_γ model, initially proposed by Lo and
90 Rao [19] and Lo and Zhang [20], by Yun et al. [9], and more recently by Thakrar et al. [12],
91 to simulate boiling flows in a vertical pipe and in a vertical rectangular channel, respectively.
92 The boiling model calculates the amount of vapour generated at the wall and the
93 corresponding mass source is added to the near-wall computational cell. Here, in the large
94 majority of CFD codes, the boundary condition on the flow field is imposed using wall
95 functions. Wall functions for use in boiling flows have been developed by different authors
96 by including, in the single-phase law of the wall, an additional roughness due to the bubbles
97 attached at the wall [8,10,14].

98 Most of the boiling models have been tested against experimental measurements made in
99 subcooled boiling flows. The majority of these experiments were performed in circular cross-
100 section geometries, with water at low pressure [13] or refrigerant at moderate pressure [21-
101 23], because they scale to typical operating conditions found in water-cooled nuclear reactors.
102 At high pressure, the availability of data is more limited and the axial averaged void profiles
103 measured by Bartlomej and Chanturiya [24] and Bartolomej et al. [25] in upward pipe water
104 flows are perhaps the most extensively investigated case to date, in addition to the DEBORA
105 experiment [22], which, instead, focused on the boiling of refrigerant R12 at moderate
106 pressures. At high pressure, the measurements of Pierre and Bankoff [26] in a rectangular
107 channel have also received some attention [12].

108 In the majority of works to date, the boiling model is tested against a single experiment and,
109 most frequently, a good predictive accuracy is demonstrated, but generally after calibration or
110 tuning of some of the model parameters to the experiment under study [7,9,10,15]. Even if
111 built in a mechanistic fashion, all the RPI-based models available at present are actually
112 forced to rely on some empirical or semi-empirical closure relation, in particular for the
113 evaporative heat transfer contribution, which requires knowledge of the active nucleation site
114 density and the bubble departure diameter and frequency. The numerous empirical
115 correlations available for this purpose were recently reviewed by Cheung et al. [27] and
116 Thakrar et al. [28]. In general, poor predictive accuracy of these models has been found for
117 subcooled boiling data over a wide range of mass and wall heat fluxes, and inlet subcooling,
118 and no combination of correlations that provide a satisfactory overall accuracy has been
119 identified. In the context of CFD, the most used correlations have been those of Lemmert and
120 Chawla [29] and Hibiki and Ishii [30] for the active nucleation site density, of Tolubinsky
121 and Kostanchuk [31] and Kocamustafaogullari [32] for the bubble departure diameter, and of
122 Cole [33] for the bubble departure frequency [7,8,10,12,16]. However, attempts to assess the
123 accuracy of these correlations for the conditions simulated are rather scarce, and no definitive
124 information on the range of parameters over which any correlation is expected to provide a
125 satisfactory accuracy, or simply outperform other correlations, is available. In view of these
126 deficiencies, some authors have recently started to use more mechanistic formulations based
127 on a balance of the forces acting on the growing bubble to calculate the bubble departure
128 diameter [9,34].

129 In this paper, a large database of subcooled boiling flows in vertical channels examined
130 experimentally over a wide range of operating conditions is assembled and predicted using a
131 model solved using the STAR-CCM+ code. It has recently been noted [35,36] how it is
132 necessary, to make progress in this field, to have models that are validated against numerous
133 experiments, rather than on a case-by-case basis which only provides good agreement with a
134 single experiment. This is particularly the case in the qualification of two-phase flow CFD
135 codes for nuclear safety applications. In view of this, changes to any model should only be
136 made if they are based on sound physical considerations, and following improvements to the
137 overall performance of the model [35,36]. In this work, a priori selected closure models are
138 applied to the whole database and the global accuracy of the model is evaluated (although
139 some changes were necessary and will be explained throughout the text). The two-phase flow
140 is described using an Eulerian-Eulerian two-fluid model, with boiling at the wall accounted
141 for using the heat flux partitioning approach. The S_7 model, based on the moments of the

142 bubble size distribution, is used to predict the bubble diameter distribution, which governs the
143 interfacial area density and therefore the interphase transfer processes. A multiphase
144 Reynolds stress turbulence model is used, which, to the authors' knowledge, represents a
145 level of closure in the context of boiling flows which has only been employed by Mimouni et
146 al. [37,38] to predict the two-phase flow in a fuel bundle subjected to the influence of a
147 mixing vane. Therefore, the impact of the use of a second-moment turbulence closure in
148 subcooled boiling simulations is further investigated. In view of the large database adopted,
149 the overall ability of multiphase CFD approaches to predict general boiling flows is
150 evaluated, this being a necessary step if models of this kind are to be confidently applied to
151 the prediction of the CHF. Areas that need further improvement are also identified and their
152 impact on the global accuracy of the model is tested. Amongst others, the multiphase
153 turbulence model and models for bubble coalescence and break-up, which are often one of
154 the weakest aspects in the simulation of bubbly flows [36], are identified.

155

156 **2 Model description**

157

158 In a two-fluid Eulerian-Eulerian model, each phase is described by a set of averaged
159 conservation equations, and the continuity, momentum and energy equations are solved for
160 each phase. These, being discussed for adiabatic two-phase boiling flows in many previous
161 publications [7,39,40] to which the interested reader may refer to, are not presented here. As
162 a consequence of the averaging procedure, details of the interphase structure are lost and
163 closure models are required for the mass, momentum and energy transfers at the interphase.
164 These, and in particular the interphase momentum exchanges, have received much attention
165 in recent years [41,42]. In this work, the drag model of Tomiyama et al. [43] is used, where
166 the drag coefficient C_D is calculated from the bubble Reynolds and Eötvös numbers, Re and
167 Eo :

168

$$C_D = \max \left[\frac{24}{Re} (1 + 0.15Re^{0.687}), \frac{8Eo}{3(Eo + 4)} \right] \quad (1)$$

169

170 A lift force, perpendicular to the direction of motion, is experienced by bubbles moving in a
171 shear flow [44] and this influences the radial void distribution in pipe and channel flows.
172 Spherical bubbles are pushed towards the pipe wall whereas larger bubbles, which are more
173 often oblate and ellipsoidal because of the inertia of the surrounding liquid, experience, after
174 a critical value of the bubble diameter, a change of sign in the lift force and accumulate

175 towards the centre of the pipe [45]. In the literature, different correlations are available for the
 176 lift coefficient that also predict the change of sign with bubble diameter [45]. The wall force,
 177 in contrast, tends to keep bubbles away from a solid wall, and was modelled first by Antal et
 178 al. [46]. Lift and wall forces in adiabatic bubbly flows are fairly well established, although
 179 some uncertainties in their effective contributions, or in the actual accuracy of the available
 180 models, still exist [47,48]. Proof of the latter is found in the numerous different models that
 181 authors have used, even in the recent past. The use of lift and wall forces in boiling flows is
 182 much more uncertain and more general studies on the behaviour of bubbles near the heated
 183 wall are necessary. In view of these uncertainties, lift and wall forces were generally
 184 neglected. The turbulent dispersion force is modelled following Burns et al. [49], with a
 185 turbulent dispersion coefficient $C_{TD} = 2.5$ and a turbulent Prandtl number $\sigma_\alpha = 1.0$ [49]:
 186

$$F_{TD} = C_{TD} \frac{3 C_D \alpha \rho_c |\mathbf{U}_r| \nu_{t,c}}{4 d_B \sigma_\alpha} \left[\frac{\nabla \alpha}{\alpha} - \frac{\nabla(1 - \alpha)}{(1 - \alpha)} \right] \quad (2)$$

187

188 **2.1 Multiphase turbulence modelling**

189

190 Turbulence is solved in the continuous phase only, with a Reynolds stress model (RSM)
 191 based on a multiphase formulation of the single-phase model due to Speziale, Sarkar and
 192 Gatsky (SSG) [50,51]:

193

$$\begin{aligned} \frac{\partial}{\partial t} \left((1 - \alpha) \rho_c R_{ij} \right) + \frac{\partial}{\partial x_j} \left((1 - \alpha) \rho_c U_{i,c} R_{ij} \right) \\ = \frac{\partial}{\partial x_j} \left[(1 - \alpha) D_{ij} \right] + (1 - \alpha) (P_{ij} + \Phi_{ij} - \varepsilon_{ij}) + (1 - \alpha) S_{ij}^{BI} \end{aligned} \quad (3)$$

194

195 Here, P_{ij} is the turbulence production, the diffusion D_{ij} is modelled accordingly to Daly and
 196 Harlow [52] and the isotropic hypothesis is used for the turbulence energy dissipation rate ε_{ij} .
 197 The pressure-strain correlation Φ_{ij} , accounting for pressure fluctuations that redistribute the
 198 turbulence kinetic energy amongst the normal Reynolds stresses, is quadratically non-linear
 199 in the anisotropy tensor [50]. In the dispersed phase, turbulence was not resolved, but was
 200 instead directly related to the turbulence of the continuous phase by means of a response
 201 coefficient C_t , assumed equal to unity [53,54] following experimental evidence that suggests
 202 such a value is reached for void fractions as low as 6 % [55].

203 With respect to a single-phase flow, the generation of turbulence by bubbles can modify
 204 significantly the turbulence in the continuous phase [56-58]. To account for this contribution,
 205 bubble-induced source terms were included in the turbulence model assuming that all the
 206 energy lost by the bubbles to drag is converted into turbulence kinetic energy inside the
 207 bubble wakes [54,59,60]:

$$S_k^{BI} = K_{BI} \mathbf{F}_d \mathbf{U}_r \quad (4)$$

208
 209
 210 The corresponding turbulence energy dissipation rate source is equal to the turbulence kinetic
 211 energy source divided by the timescale of the bubble-induced turbulence, calculated from the
 212 velocity scale of the turbulence and the length scale of the bubbles [60]:

$$S_\varepsilon^{BI} = C_{\varepsilon,BI} \frac{S_k^{BI}}{\tau_{BI}} = 1.0 \frac{k^{0.5}}{d_B} S_k^{BI} \quad (5)$$

213
 214
 215 The mixed timescale, used in combination with the coefficient $K_{BI} = 0.25$, has been found to
 216 provide accurate predictions over a wide range of bubbly pipe flows [61]. The need for a
 217 bubble-induced turbulence contribution in bubbly flows has been demonstrated in many
 218 previous studies [48,54,60]. In contrast, less established is the use of these bubble-induced
 219 turbulence models in boiling flows and, therefore, this specific issue is further discussed in a
 220 specific section within the Results and discussion.

221 222 **2.2 The S_γ model**

223
 224 Bubbles, after departure from the heated wall, experience evaporation and condensation in
 225 the bulk of the flow, and break-up and coalescence events that alter the bubble diameter
 226 distribution and affect the interphase mass, momentum and energy exchanges. The bubble
 227 diameter distribution is predicted with the S_γ model [19,20], where it is assumed to obey to a
 228 pre-defined log-normal probability distribution $P(d_B)$. From this, the density of the moments
 229 of the bubble size distribution M_γ may be derived:

$$S_\gamma = nM_\gamma = n \int_0^\infty d_B^\gamma P(d_B) d(d_B) \quad (6)$$

230
 231

232 The zeroth order moment is equal to the bubble number density n , whereas S_2 and S_3 are
 233 closely related to the interfacial area concentration and the void fraction:

234

$$S_0 = n; S_2 = n \int_0^\infty d_B^2 P(d_B) d(d_B) = \frac{a_i}{\pi}; S_3 = n \int_0^\infty d_B^3 P(d_B) d(d_B) = \frac{6\alpha}{\pi} \quad (7)$$

235

236 Average diameters of different kinds of bubble are obtained by combining the moment
 237 densities, including, from S_2 and S_3 , the Sauter-mean diameter (SMD), which is compared
 238 against experiments later:

239

$$d_{SM} = d_{32} = \frac{S_3}{S_2} = \frac{6\alpha}{a_i} \quad (8)$$

240

241 Additionally, the variance of the distribution is calculated from:

242

$$\sigma^2 = \ln\left(\frac{d_{32}}{d_{30}}\right) = \ln\left[\frac{(S_3/S_2)}{(S_3/S_0)^{1/3}}\right] \quad (9)$$

243

244 The two average diameters, d_{32} and d_{30} , are equal only for a monodispersed distribution.
 245 Since the void fraction is known from the two-fluid model, the solution of only two
 246 additional equations for S_0 and S_2 is sufficient to characterize the bubble size distribution. For
 247 each moment, a transport equation of the following type needs to be solved:

248

$$\frac{\partial S_\gamma}{\partial t} + \nabla \cdot (S_\gamma \mathbf{U}_v) = S_{br} + S_{cl} + S_m \quad (10)$$

249

250 The source terms account for the contributions of bubble break-up and coalescence, with the
 251 last being the source due to boiling at the wall and condensation/evaporation in the bulk of
 252 the flow:

253

$$S_m = N d_w^\gamma + \frac{2 S_2 m_{lv}}{3 \rho_v \alpha} \quad (11)$$

254

255 In this work, interactions induced by turbulence were assumed to be dominant and the only
 256 mechanism inducing break-up and coalescence events [6,20]. The source term for bubble
 257 break-up is expressed as:

$$258 \quad S_{br} = \int_0^{\infty} K_{br} \Delta S_{\gamma}^{br} n P(d_B) d(d_B) \quad (12)$$

259 where K_{br} is the break-up rate, the reciprocal of the break-up time τ_{br} , and ΔS_{γ}^{br} is the change
 260 in S_{γ} due to a single break-up event, which, from conservation of volume, is:
 261

$$262 \quad \Delta S_{\gamma}^{br} = d_B^{\gamma} \left(N_f^{\frac{3-\gamma}{\gamma}} - 1 \right) \quad (13)$$

263 The number of daughter bubbles N_f was assumed equal to 2 [6,20,62]. The break-up
 264 timescale follows from the frequency of the second oscillation mode of a droplet [20]:
 265

$$266 \quad \tau_{br} = 2\pi k_{br} \sqrt{\frac{3\rho_d + 2\rho_c}{192\sigma}} d_B^3 \quad (14)$$

267 with $k_{br} = 0.2$. Bubbles break when the Weber number is higher than a critical value We_{crit} ,
 268 equal to 1.24 [6,48]:
 269

$$270 \quad d_{crit} = (1 + C_{\alpha}) \left(\frac{2\sigma We_{crit}}{\rho_c} \right)^{3/5} \varepsilon^{-2/5} \quad (15)$$

271 C_{α} , equal to 4.6, is a correction factor that accounts for nearby bubbles that disrupt the
 272 influence of the surrounding inertial forces. The general source term for bubble coalescence
 273 is:
 274

$$275 \quad S_{cl} = \int_0^{\infty} \int_0^{\infty} K_{cl}^{d,d'} \Delta S_{\gamma,cl}^{d,d'} n^2 P(d') d(d') P(d) d(d) \quad (16)$$

276 Here, $K_{cl}^{d,d'}$ is the coalescence rate between two bubbles with diameters d and d' , and $\Delta S_{\gamma,cl}^{d,d'}$
 277 is the change in S_{γ} due to a single coalescence event. Following [20], and to avoid excessive
 278

279 computational cost, it is assumed, in the coalescence source term, that the bubble diameter
 280 has a uniform distribution with an equivalent mean diameter, taken equal to the SMD.
 281 Therefore, the change in S_γ due to a single coalescence event becomes:

$$282 \quad \Delta S_{\gamma,cl}^{d,d'} = d_{SM}^\gamma (2^{\gamma/3} - 2) \quad (17)$$

283
 284 From Yao and Morel [6], the number of coalescence events per unit volume and unit time is
 285 expressed as:

$$286 \quad K_{cl}^{d,d'} n^2 = -C_1 \frac{\varepsilon^{1/3} \alpha^2}{d_{SM}^{11/3}} \frac{1}{g(\alpha) + C_2 \sqrt{We/We_{crit}}} \exp\left(-C_3 \sqrt{We/We_{crit}}\right) \quad (18)$$

287
 288 The first part of Eq. (18) represents the collision rate between the bubbles, whilst the
 289 exponential function describes the probability of coalescence following a collision event. The
 290 function $g(\alpha)$ accounts for the effect of the packing of the bubbles when the void fraction is
 291 higher than a certain value. From [6], $C_1 = 2.86$, $C_2 = 1.922$, $C_3 = 1.017$ and $We_{crit} = 1.24$.

292 2.3 Boiling model

293
 294 When boiling occurs at a heated wall, different heat transfer mechanisms take place and these
 295 need to be modelled. In regions of the wall where no bubbles are growing, the heat is
 296 transferred to the liquid by single-phase convection. Otherwise, the heat is removed by the
 297 evaporation process and supports the growth of bubbles at the nucleation sites. Bubbles grow
 298 attached to the wall until, when certain conditions are reached, detachment occurs.
 299 Detachment of bubbles promotes additional mixing in the fluid phase and the recirculation of
 300 subcooled liquid which is brought into contact with the wall to fill the volume which was
 301 previously occupied by the detaching bubble. This mechanism accounts for a portion of the
 302 heat transferred from the wall, and is known as quenching. Finally, when a significant
 303 amount of vapour is present at the wall, liquid access to the wall may be restricted and a
 304 portion of the heat is transferred by convection to the vapour phase. Therefore, and following
 305 the RPI model of Kurul and Podowski [5], the total heat transferred from the wall is
 306 partitioned between these heat transfer mechanisms:

$$307 \quad Q_w = (Q_l + Q_q + Q_{ev})(1 - K_{dry}) + K_{dry} Q_v \quad (19)$$

309

310 K_{dry} is the fraction of the wall in contact with the vapour which becomes larger than zero
311 when the void fraction is higher than a critical value, assumed equal to 0.9 [51]. The single-
312 phase convective volumetric heat flux to the liquid phase is obtained from:

313

$$Q_l = (1 - A_b) \frac{\rho_l C_{p,l} u_{\tau,l}}{T_l^+} (T_w - T_l) \quad (20)$$

314

315 A_b is the fraction of the wall influenced by the evaporation process and T^+ a dimensionless
316 temperature, which is calculated using the wall function approach [51]. In the same way, the
317 convective volumetric heat flux to the vapour phase is known from:

318

$$Q_v = \frac{\rho_v C_{p,v} u_{\tau,v}}{T_v^+} (T_w - T_v) \quad (21)$$

319

320 The quenching volumetric heat flux, which accounts for the additional heat transfer to the
321 cooler liquid that replaces a bubble detaching from the wall, is given by:

322

$$Q_q = h_q (T_w - T_l) \quad (22)$$

323

324 The quenching heat transfer coefficient is modelled accordingly to Del Valle and Kenning
325 [63]:

326

$$h_q = 2A_b f \sqrt{\frac{\rho_l C_{p,l} \lambda_l t_w}{\pi}} \quad (23)$$

327

328 In the previous equation, t_w is the waiting time between the bubble departure and the
329 nucleation of the next bubble:

330

$$t_w = \frac{0.8}{f} \quad (24)$$

331

332 In Eq. (22), and to avoid any dependency on the computational grid employed, the liquid
333 temperature is evaluated at a constant y^+ of 250.

334 The evaporative volumetric heat flux is known from the number of bubbles that grow
 335 attached to the heated wall at the active nucleation sites. These bubbles grow until the forces
 336 that promote detachment overcome those that keep the bubble attached to the wall. Therefore,
 337 the evaporative heat flux is known from the number of active nucleation sites, the diameter of
 338 the bubbles at departure and the frequency of the bubble departure from the wall:

$$339 \quad Q_{ev} = n' f \left(\frac{\pi d_w^3}{6} \right) \rho_v i_{lv} \quad (25)$$

340
 341 In Eq. (25), closure relations are required for the nucleation site density, the bubble departure
 342 diameter and the bubble departure frequency. Most often, these have been obtained from
 343 empirical correlations. Only recently have more mechanistic formulations been introduced to
 344 calculate the bubble departure diameter [9,34]. In this work, two correlations for both the
 345 nucleation site density and for the bubble departure diameter are considered. Lemmert and
 346 Chawla [29] proposed correlating the nucleation site number density to the wall superheat:

$$347 \quad n' = n_0 (T_w - T_{sat})^p \quad (26)$$

348
 349 with $n_0 = 12366.45 \text{ m}^{-2}\text{K}^{-1}$ and $p = 1.805$. More recently, it has become evident that, to have a
 350 model with a wide applicability, correlation to other parameters has to be taken into account,
 351 including properties of the heated surface such as the contact angle [30]. The more recent
 352 model from Hibiki and Ishii [30] is given by:

$$353 \quad n' = n_0 \left[1 - \exp\left(-\frac{\theta^2}{8\mu'^2}\right) \right] \left[\exp\left(f' \frac{\lambda'}{R_c}\right) - 1 \right] \quad (27)$$

354
 355 where $n_0 = 4.72 \times 10^5 \text{ m}^{-2}$, $\mu' = 0.722 \text{ rad}$ and $\lambda' = 2.50 \times 10^{-6} \text{ m}$. θ is the contact angle, f' a
 356 function of $\rho^+ = \log(\Delta\rho / \rho_v)$ and R_c is equal to:

$$357 \quad R_c = \frac{2\sigma[1 + \rho_v/\rho_l]/p}{\exp[i_{lv}(T_v - T_{sat})/R_g T_v T_{sat}] - 1} \quad (28)$$

358
 359 Tolubinsky and Kostanchuk [31] correlated the bubble departure diameter to the liquid
 360 subcooling:

361

$$d_w = d_0 \exp[-(T_{sat} - T_l)/\Delta T_0] \quad (29)$$

362

363 Here, $d_0 = 0.0006$ m and $\Delta T_0 = 45$ K. Kocamustafaogullari [32] developed a model for the
364 bubble departure diameter based on a balance between gravity and surface tension forces.
365 The model, with the addition of the dependency on a density ratio, was developed to account
366 for the effect of the system pressure:

367

$$d_w = d_l \theta \left(\frac{\sigma}{g\Delta\rho} \right)^{0.5} \left(\frac{\Delta\rho}{\rho_v} \right)^{0.9} \quad (30)$$

368

369 where $d_l = 1.5126 \times 10^{-3}$ m rad⁻¹ and $\theta = 0.722$ rad for water systems. The bubble departure
370 frequency is calculated from Cole [33]:

371

$$f = \sqrt{\frac{4}{3} \frac{g(\rho_l - \rho_v)}{d_w \rho_l}} \quad (31)$$

372

373 The fraction of the wall affected by the evaporation process is known from [5]:

374

$$A_b = 2.0 \frac{\pi d_w^2}{4} n' \quad (32)$$

375

376 Finally, in the bulk of the fluid, the liquid side heat transfer coefficient at the interphase is
377 calculated using the Ranz and Marshall [64] correlation:

378

$$h_l = \frac{\lambda_l}{d_B} (2 + 0.6Re^{1/2}Pr^{1/3}) \quad (33)$$

379

380 The overall model, implemented in the STAR-CCM+ CFD code [51], is solved in a two-
381 dimensional axisymmetric geometry. At the inlet, fully-developed single-phase liquid
382 velocity, turbulence and temperature are imposed, together with an imposed pressure at the
383 outlet and the no-slip condition, and an imposed heat flux, at the wall. Strict convergence of
384 residuals was ensured, together with a mass balance error always lower than 0.01 % for both
385 phases. A mesh sensitivity study demonstrated that grid-independent solutions were achieved

386 with an equidistant structured mesh with the first grid point placed at a minimum wall
387 distance of $y^+ = 30$, which is the lower limit for the use of wall functions.

388

389 **3 Experimental data**

390

391 Confidence in the predictions of CFD codes relies on extensive validation of their results
392 against relevant experimental data. In this regard, it is important that models provide accurate
393 predictions over many experiments, with parameter variations as wide as possible. Therefore,
394 a database was built from 20 experiments from 5 different sources: Bartolomej and Chanturiya
395 [24], Bartolomej et al. [25], Roy et al. [21], the DEBORA experiment [22] and Lee et al. [13].
396 The database, which is summarized in Table 1, includes measurements in vertical pipes and
397 annular channels of subcooled boiling flows of water, Freon-12 and refrigerant R-113, and
398 covers the ranges 0.101 – 6.89 MPa for the pressure, 477 – 2981 kg m⁻²s⁻¹ for the mass flux,
399 58.2 – 1200 kW m⁻² for the heat flux and 11.5 – 63 °C for the inlet subcooling.

400 The DEBORA [22] flow loop consisted of a 19.2 mm inner diameter vertical pipe, heated for
401 a length of 3.5 m and operated with Freon-12 (R-12). Given the inherent difficulties of
402 measuring the flow boiling of water at high pressure, and temperature, Freon-12 guaranteed
403 more favourable experimental conditions, while maintaining values of dimensionless groups
404 such as the Reynolds and the Weber number, and the density ratio, consistent with typical
405 operating conditions of pressurized water reactors. Measurements were taken in the ranges
406 1.46 – 3.01 MPa for the pressure, 1000 – 3000 kg m⁻²s⁻¹ for the mass flux and 58 – 135 kW
407 m⁻² for the heat flux, and a significant range of liquid subcooling. Void fraction and vapour
408 velocity profiles at the end of the test section were measured with an optical probe technique,
409 from which radial profiles of the interfacial area concentration and the SMD were
410 determined. Thermocouples were used to measure the liquid temperature radial profile and
411 the wall temperature at selected axial locations.

412 Bartolomej and Chanturiya [24], and Bartolomej et al. [25], investigated the subcooled boiling
413 of water in vertical pipes of inlet diameter $D = 0.0154$ m and 0.012 m, and length $L = 2$ m
414 and 1.4 m, respectively. Average void fractions were measured at different axial locations at
415 pressures up to 15 MPa, mass fluxes up to 2000 kg m⁻²s⁻¹ and heat fluxes up to 2.2 MW m⁻².
416 For this study, five cases were selected from these experiments at pressures up to 6.89 MPa,
417 mass fluxes up to 1500 kg m⁻²s⁻² and heat fluxes up to 1.2 MW m⁻² (Table 1).

418 Roy et al. [21] tested the subcooled boiling of refrigerant R-113 in a vertical annulus of 3.66
419 m in length, 0.0158 m in inlet diameter and 0.0381 m in outlet diameter. A laser Doppler

420 velocimetry system allowed measurement of the velocity field and the turbulent fluctuations,
421 with an optical probe used to obtain the void fraction and the bubble diameter. The liquid and
422 vapour temperatures were measured with micro-thermocouples. Measurements were taken at
423 0.269 MPa and in the ranges 565 – 785 kg m⁻²s⁻¹ for the mass flux, 79.4 – 125.9 kW m⁻² for
424 the heat flux and 42.7 – 50.2 °C for the inlet temperature. In a slightly different annular
425 channel, 2.376 m in length, 0.019 m in inlet diameter and 0.0375 m in outlet diameter, Lee et
426 al. [13] investigated the subcooled flow boiling of water at nearly atmospheric pressure, and
427 474 – 1061 kg m⁻²s⁻¹ for the mass flux, 115 – 300 kW m⁻² for the heat flux and 11.5 – 21.3 °C
428 for the inlet subcooling. Liquid velocity radial profiles were measured with a Pitot tube, and
429 vapour velocity and void fraction radial profiles with a two-conductivity probe method.
430 None of the previous experiments provides a complete characterization of the flow, which is
431 a shortcoming of most of the experimental data available to date. Limited measurements of
432 the bubble diameter are available from Roy et al. [21] and, therefore, the DEBORA
433 experiment is the only one that provides radial profiles of the average bubble diameter.
434 However, in the DEBORA experiment, liquid velocity profiles and liquid turbulence profiles
435 were not measured. Turbulence profiles, in particular, are only available from Roy et al. [21].
436 Temperatures were measured in the DEBORA and the Roy et al. [21] experiments, but not by
437 Lee et al. [13], which also did not provide any information on liquid turbulence and bubble
438 diameter. Finally, in Bartolomej and Chanturiya [24] and Bartolomej et al. [25], and since
439 these experiments were undertaken at higher pressures and some decades ago, only the
440 average void fraction at different axial locations was measured. Even so, these experiments
441 are one of the few to give measurements at high pressure. The use of a large database
442 therefore overcame the limitation of each individual dataset, allowing validation of the model
443 for all physical quantities of interest. It is important to note, however, the necessity for more
444 detailed and comprehensive experimental data sets in order to improve our ability to predict
445 these kinds of flows, since, as will be seen in the following section, the parameters of interest
446 interact with each other in a rather complex and non-linear way.

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Table 1. Summary of the experimental conditions included in the validation database.

Data	Source	p [MPa]	p _r [-]	G [kg m ⁻² s ⁻¹]	q'' [kW m ⁻²]	T _{in} [°C]	Fluid	Geometry
deb1	Garnier et al. [22]	2.62	0.63	1996	73.9	68.5	R12	P
deb2	Garnier et al. [22]	2.62	0.63	1985	73.9	70.5	R12	P
deb3	Garnier et al. [22]	1.46	0.35	2023	76.3	39.7	R12	P
deb4	Garnier et al. [22]	1.46	0.35	2028	76.2	34.9	R12	P
deb5	Garnier et al. [22]	2.62	0.63	2981	109.4	69.2	R12	P
deb6	Garnier et al. [22]	3.01	0.73	1007	58.2	64.6	R12	P
roy1	Roy et al. [21]	0.269	0.08	565	79.4	42.7	R113	A
roy2	Roy et al. [21]	0.269	0.08	785	95.0	50.2	R113	A
roy3	Roy et al. [21]	0.269	0.08	785	125.9	50.2	R113	A
lee1	Lee et al. [13]	atm	0.005	478	152.8	80.8	W	A
lee2	Lee et al. [13]	atm	0.005	477	114.8	88.5	W	A
lee3	Lee et al. [13]	atm	0.005	718	232.6	78.8	W	A
lee4	Lee et al. [13]	atm	0.005	714	197.2	86.2	W	A
lee5	Lee et al. [13]	atm	0.005	1061	300.0	81.9	W	A
lee6	Lee et al. [13]	atm	0.005	1047	251.2	86.6	W	A
bar1	Bartolomej and Chanturiya [24]	1.5	0.07	900	380	138.3	W	P
bar2	Bartolomej and Chanturiya [24]	4.5	0.20	900	570	197.4	W	P
bar3	Bartolomej et al. [25]	6.89	0.31	1500	1200	221.9	W	P
bar4	Bartolomej et al. [25]	6.89	0.31	1500	800	245.9	W	P
bar5	Bartolomej et al. [25]	6.89	0.31	1000	800	229.9	W	P

456 atm = atmospheric; W = water; P = pipe; A = annular channel.

457

458 4 Results and discussion

459

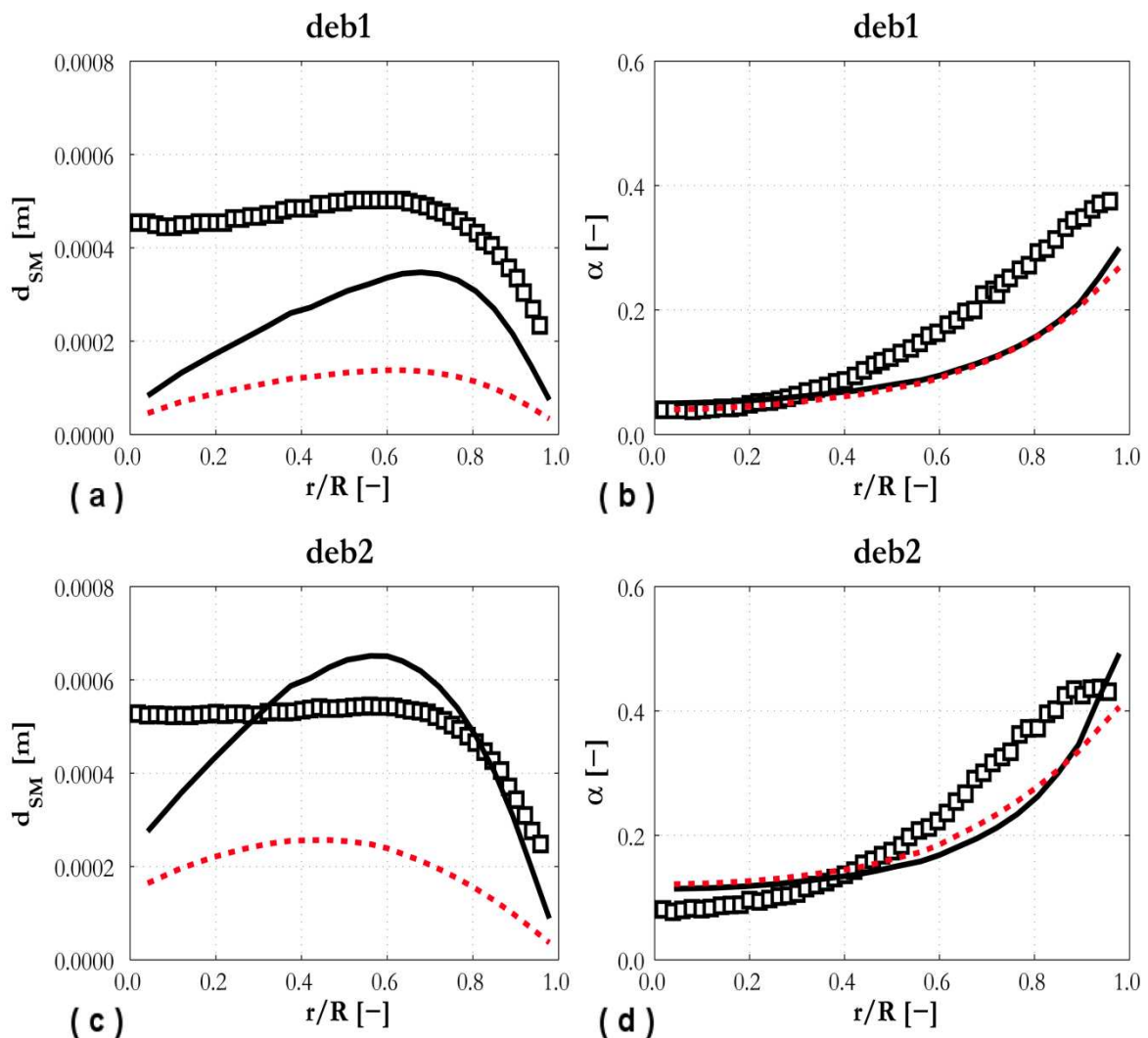
460 4.1 Coalescence source

461

462 Before simulating the whole database, some model parameters had to be selected, starting
 463 with the coalescence source, calculated from Yao and Morel [6]. In a previous work, a critical
 464 Weber number $We_{crit} = 0.10$ in the coalescence efficiency allowed good agreement to be
 465 obtained for different air-water bubbly flows in vertical pipes [65]. This agreement was
 466 achieved in combination with the assumption of negligible bubble break-up, which is
 467 expected to be even lower in boiling flows due to the lower expected bubble diameter. In
 468 bubbly flow experiments, therefore, bubbles are usually injected with a diameter of the order
 469 of a few millimetres. In contrast, during boiling, bubbles may detach from the wall with a
 470 diameter up to one or two orders of magnitude smaller.

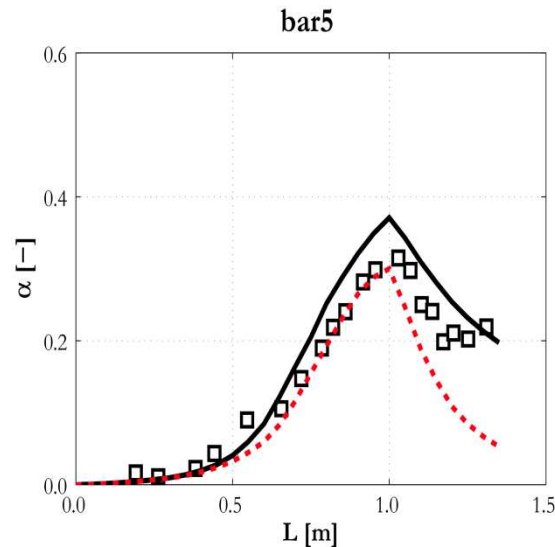
471 Yao and Morel [6] proposed a value of 1.24 for We_{crit} , rather higher than the value of 0.1
 472 adopted in [65]. These two values are compared for the deb1 and deb2 experiments (see
 473 Table 1) in Figure 1. In the plots, profiles of the SMD and the void fraction are shown as a
 474 function of the normalized radial distance, with the centre of the pipe located at $r/R = 0.0$ and
 475 the wall at $r/R = 1.0$. As expected, We_{crit} has a significant impact on the SMD radial profile.
 476 More specifically, $We_{crit} = 0.10$ leads to a large underestimation of the SMD, probably as a
 477 consequence of weak bubble coalescence in the flow. With $We_{crit} = 1.24$, the SMD is still
 478 under predicted in deb1 (Figure 1a), although the agreement is improved. For deb2, the

479 results are more in line with the experimental measurements (Figure 1c). Relative to the
 480 SMD, other variables are less affected by the amount of coalescence, this being the case in
 481 Figure 1 for the void fraction radial profiles (Figure 1b and Figure 1d). To provide a further
 482 evaluation, experiment bar5 was also simulated and the axial distribution of the cross-
 483 sectional averaged void fraction is shown in Figure 2. In this case, the difference between the
 484 simulation results is more marked, with lower coalescence in the flow causing a lower
 485 average void fraction, probably as a consequence of the higher condensation. The
 486 condensation heat transfer coefficient is indeed inversely proportional to the bubble diameter.
 487 In view of these results, $We_{crit} = 1.24$ was selected for the following simulations.
 488



489
 490 Figure 1. SMD and void fraction radial profiles compared against experiments deb1 (a,b) and
 491 deb2 (c,d) and for different values of We_{crit} in the coalescence model: (—) 1.24; (---) 0.1.

492
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 494



495
 496 Figure 2. Average void fraction axial development compared against experiment bar5 and for
 497 different values of We_{crit} in the coalescence model: (—) 1.24; (---) 0.1.

498
 499 **4.2 Bubble departure diameter**

500
 501 In preliminary simulations, it was found impossible to use, in the boiling model, the same set
 502 of closure relations to address the entire database, in particular for the active nucleation site
 503 density and the bubble departure diameter. For the nucleation site density, the Hibiki and Ishii
 504 model [30] was maintained for the entire database because it accounts for the effect of more
 505 parameters. Due to the fact that the database extends from atmospheric pressure up to 6.89
 506 MPa, the Kocamustafaogullari model [32] was initially considered for the bubble departure
 507 diameter, this being derived over the range $0.0067 < p < 14.18$ MPa. In contrast, the
 508 Tolubinsky and Kostanchuk [31] correlation was derived for $0.1 < p < 1.013$ MPa and 0.08
 509 $< U_l < 0.20$ m s⁻¹ and has a pressure insensitive formulation, with the bubble departure
 510 diameter being only a function of the bulk subcooling. Unfortunately, using the
 511 Kocamustafaogullari correlation [32], reliable results were not obtained for the Roy et al. [21]
 512 data and the experiments of Bartolomej and co-authors [24,25]. An example is provided in
 513 Figure 3, which shows predictions of the void distribution given by this correlation for the
 514 bar2 (Figure 3b) and the bar4 (Figure 3d) experiments and compares these with the results
 515 obtained using the Tolubinsky and Kostanchuk [31] correlation (Figure 3a and Figure 3c,
 516 respectively). In the figure, $r/R = 0.0$ corresponds to the pipe axis and $r/R = 1.0$ to the pipe
 517 wall. For bar2, at 4.5 MPa, Kocamustafaogullari [32] predicts a void fraction that is
 518 comparable with that from Tolubinsky and Kostanchuk [31]. At higher pressure (bar4, 6.89
 519 MPa), however, the void fraction predicted with Kocamustafaogullari [32] is almost
 520 negligible, except for a very thin portion of the wall region. Therefore, due to the negligible

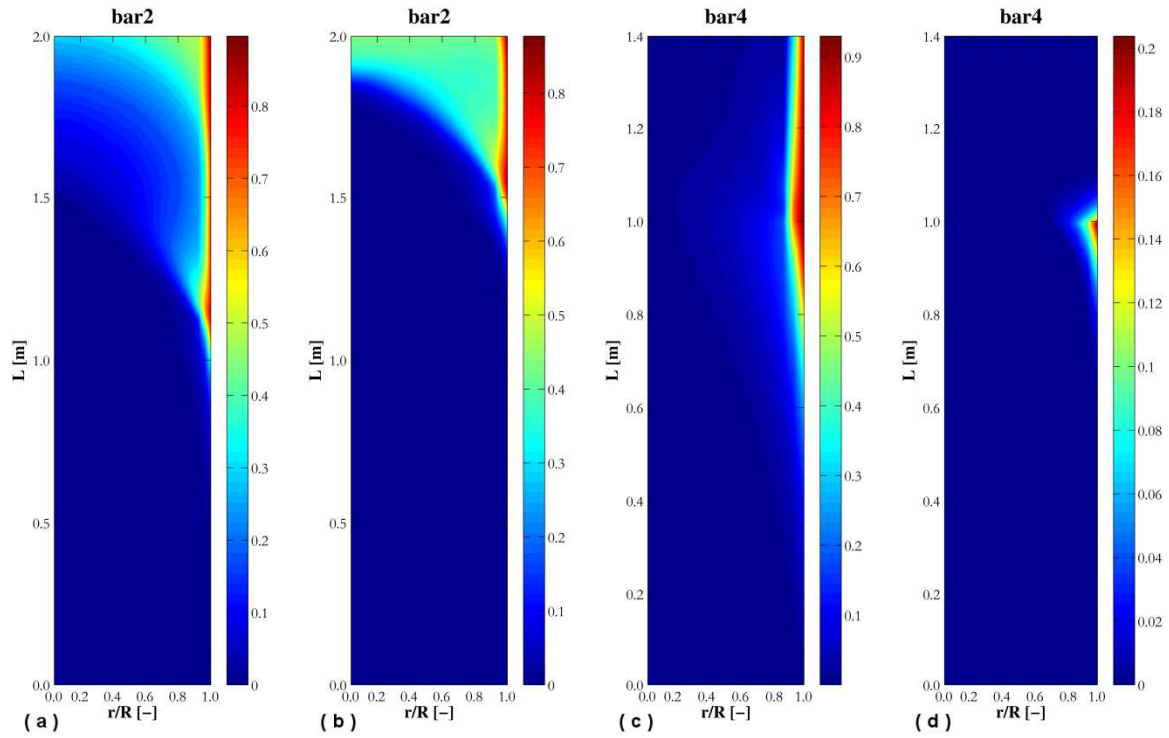
521 evaporation predicted in some of the experiments, for the data of Bartolomej and Chanturiya
522 [24], Bartolomej et al. [25] and Roy et al. [21], the Tolubinsky and Kostanchuk [31]
523 correlation was used.

524 To investigate the subject further, some bubble departure diameter data selected from the
525 literature was tested against the Kocamustafaogullari model [32]. These data were taken from
526 Unal et al. [66] for water at high pressure, and from Klausner et al. [67] and Zeng et al. [68]
527 who used refrigerant R113, as employed by Roy et al. [21], at atmospheric pressure.
528 Percentage relative errors between predictions and data are shown in Figure 4. In general, the
529 bubble departure diameter is under predicted. More specifically, 50 – 75 % smaller diameters
530 are found for refrigerant R113 and, for water, the departure diameter is overestimated at low
531 pressure, but under predicted by up to 100% at high pressure. Overall, the relative percentage
532 errors are rather high, therefore the model cannot be considered reliable over a wide range of
533 conditions.

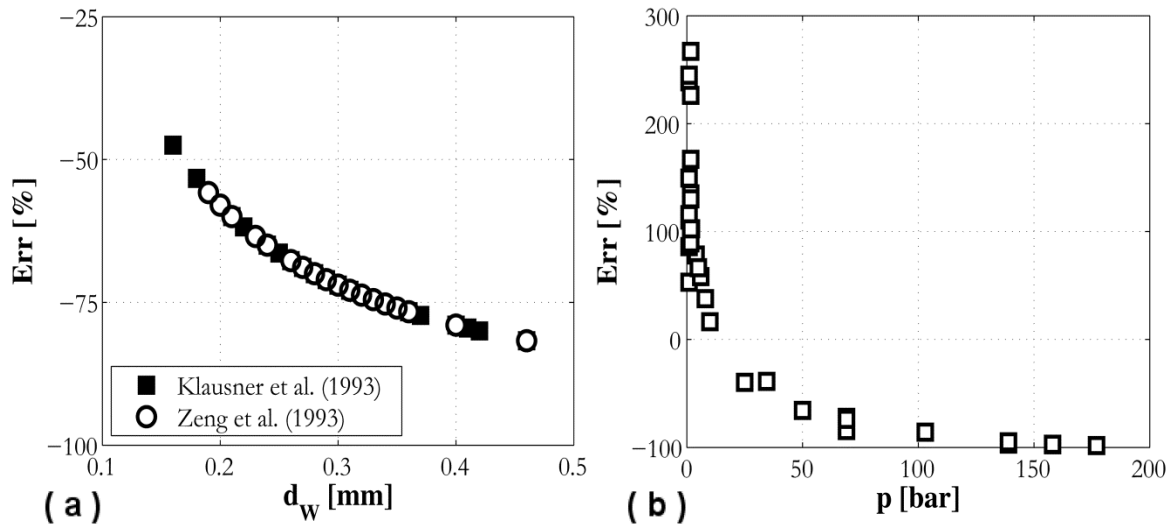
534 In line with the approach of the paper, it would have been desirable to maintain the
535 Tolubinsky and Kostanchuk [31] correlation for the whole database. However, this
536 correlation is also not entirely reliable even given its range of validity, as it was found that
537 unrealistically large bubbles were predicted by it for some of the Lee et al. [13] and the
538 DEBORA [22] experiments at low pressure, which prevented convergence of the simulations.
539 Therefore, for these two databases, the Kocamustafaogullari [32] correlation was used.

540

541



542 Figure 3. Void fraction radial distribution along the pipe for bar2 and bar4 experiments: (a,c)
 543 Tolubinsky and Kostanchuk [31] bubble departure diameter correlation; (b,d)
 544 Kocamustafaogullari [32] bubble departure diameter correlation.
 545
 546
 547



548 Figure 4. Relative percentage error for the Kocamustafaogullari [32] bubble departure
 549 diameter correlation compared against: (a) Klausner et al. [67] and Zeng et al. [68] for
 550 refrigerant R113; (b) Unal et al. [66] for water at different pressures.
 551
 552
 553

554 4.3 Comparison with the entire database

555

556 After the preliminary selection of some of the model parameters, the overall model was
557 applied to the whole database without further modification. Comparisons for the DEBORA
558 experiments are presented in Figure 5 and Figure 6, and in Figure 7 for Roy et al. [21], in
559 Figure 8 for Lee et al. [13] and in Figure 9 for Batolomej and Chanturiya [24] and Bartolomej
560 et al. [25]. In these, and subsequent figures, symbols are used for experimental data and lines
561 for model predictions. In annular channels (Figure 7 and Figure 8), the radial position is non-
562 dimensionalized with the distance between the outer and inner radius and, therefore, in the
563 plots $(r - R_i) / (R_o - R_i) = 0.0$ identifies the inner wall, whereas $(r - R_i) / (R_o - R_i) = 1.0$
564 corresponds to the outer wall. Only the inner wall is heated in both the Roy et al. [14] and the
565 Lee et al. [13] experiments. In the following, discussion of the results is presented for each
566 physical quantity predicted.

567

568 4.3.1 Void fraction

569 Even if the specific quantitative accuracy depends on the particular experiment, the void
570 fraction profile is generally predicted with reasonable accuracy. More specifically, the
571 accuracy is satisfactory for the DEBORA experiment (Figure 5 and Figure 6), but with the
572 exception of deb6 (Figure 6c) where the void profile is significantly under predicted. Also, an
573 over predicted void peak at the heated wall was obtained for deb4 (Figure 6a). For deb3, it
574 must be remarked that the void fraction profile (Figure 5j) is core-peaked and the bubble
575 diameter (Figure 5k) higher than in all the other experiments. It is known from the literature
576 that larger bubbles assume ellipsoidal shapes, being deformed by the inertia of the
577 surrounding liquid, and are pushed towards the centre of the pipe by a negative lift force [45].
578 In this experiment, bubbles may have been large enough to trigger the change of sign in the
579 lift force and, even if wall-peaked void profiles were predicted neglecting the lift
580 contribution, a negative lift was necessary to predict the void profile. In Figure 7, void
581 fraction profiles are well predicted for Roy et al. [21], the only discrepancy being a minor
582 underestimation in the case of roy3. In contrast, the void fraction tends to be underestimated
583 in the experiments of Lee et al. [13] (Figure 8). More specifically, the predicted void fraction
584 is in agreement with experiment or over predicted near the wall, whereas it is underestimated
585 in the remainder of the pipe. The best results are obtained at the lowest mass flux (lee1 in
586 Figure 8a and lee2 in Figure 8c), and the largest errors in lee5 (Figure 8i). Lastly, in the
587 Bartolomej and co-authors' experiments [24,25], only the averaged axial void distribution

588 was available and this is well predicted for bar1 and bar2 (Figure 9a), apart from a divergence
589 at around 1.25 m in bar2. Reasonable agreement is found for the Bartolomej et al. [25]
590 experiments in Figure 9b, despite the slight over prediction in bar3 and bar5.

591

592 **4.3.2 Sauter-mean diameter**

593 Measurements of the SMD were available for the DEBORA experiments only. Overall, the
594 model under predicts the experiments, in particular near the centre of the pipe, although
595 reasonable agreement is achieved for experiments deb2 (Figure 5g) and deb3 (Figure 5k),
596 whereas the under prediction is particularly large in deb6 (Figure 6e). In more detail, the
597 SMD is underestimated close to the heated wall and, after a partial improvement in the first
598 region away from the wall, predictions decrease significantly towards the pipe axis. In
599 contrast, the experimental profiles tend to remain nearly flat towards the centre of the pipe. In
600 deb3 (Figure 5k), the SMD increases towards the pipe centre, most likely as a consequence of
601 the core-peaked void fraction profile in this experiment, a trend that is also predicted by the
602 simulation. Overall, the significant discrepancies with the experiments may be due to a
603 number of different factors, the individual impact of which is difficult to quantify. Certainly,
604 the interphase heat transfer coefficient and the models for coalescence and break-up may play
605 a role that needs to be investigated further. In addition, the underestimation of the SMD in the
606 wall region suggests a significant impact of the bubble departure diameter correlation. This,
607 in conjunction with the unreliability of each bubble departure correlation over a wide range of
608 conditions, discussed in Section 4.2, demonstrates how the development of more advanced,
609 mechanistic formulations of the bubble departure diameter is a priority for further research.

610

611 **4.3.3 Liquid temperature**

612 Liquid temperature profiles were measured by Roy et al. [21] and in the DEBORA
613 experiments. Overall, predictions are in good agreement with data. For the DEBORA
614 experiments, the flat temperature profile for deb2 (Figure 5h) and deb3 (Figure 5l) indicates a
615 flow close to saturation that may have helped to limit the underestimation of the SMD for
616 these experiments (Figure 5g and Figure 5k). deb1 (Figure 5d), instead, shows a slightly
617 higher degree of subcooling near the axis. The Roy et al. [21] experiments (Figure 7d, Figure
618 7h and Figure 7l), which exhibit a higher degree of subcooling away from the wall, are also

619 well predicted, despite the temperature being slightly over estimated close to the wall and
620 under estimated near the axis.

621

622 **4.3.4 Velocity profiles**

623 Liquid and vapour average velocities were measured by Roy et al. [21] and Lee et al. [13],
624 whereas only the average vapour velocity profile is available for the DEBORA experiments.
625 The vapour velocity profile is very well predicted for deb3 (Figure 5i), although for deb1
626 (Figure 5a) and deb2 (Figure 5e), the profile remains flat near the pipe centre, probably as a
627 consequence of the lower value of the SMD in this region. However, predictions may be
628 considered satisfactory for these pipe flows. On the other hand, the predicted accuracy is
629 unsatisfactory in the annular channels of Roy et al. [21] and Lee et al. [13]. More specifically,
630 both predicted velocity profiles show a peak at the wall that is in contrast found away from
631 the wall in the experiments (Figure 7b, Figure 7f, Figure 7j, Figure 8b, Figure 8d, Figure 8f,
632 Figure 8h, Figure 8j and Figure 8l). This phenomenon is even more evident in the vapour
633 velocity profiles. Away from the wall, in particular for Roy et al. [21], the velocity profiles
634 are more in agreement with the experiments. The peak away from the wall is explained due to
635 the presence, in this region, of larger bubbles that flow with a higher relative velocity. In Lee
636 et al. [13], probably as a consequence of the atmospheric pressure that promotes the growth
637 of even larger bubbles, these peaks are sometimes found in the “unheated half” of the
638 channel. In the simulations, however, the SMD peaks at the wall and the model is unable to
639 correctly account for the presence of the larger bubbles, with this inability also contributing
640 to the low SMD values and the flat velocity profiles in the centre of the channel predicted in
641 deb1 (Figure 5a) and deb2 (Figure 5e).

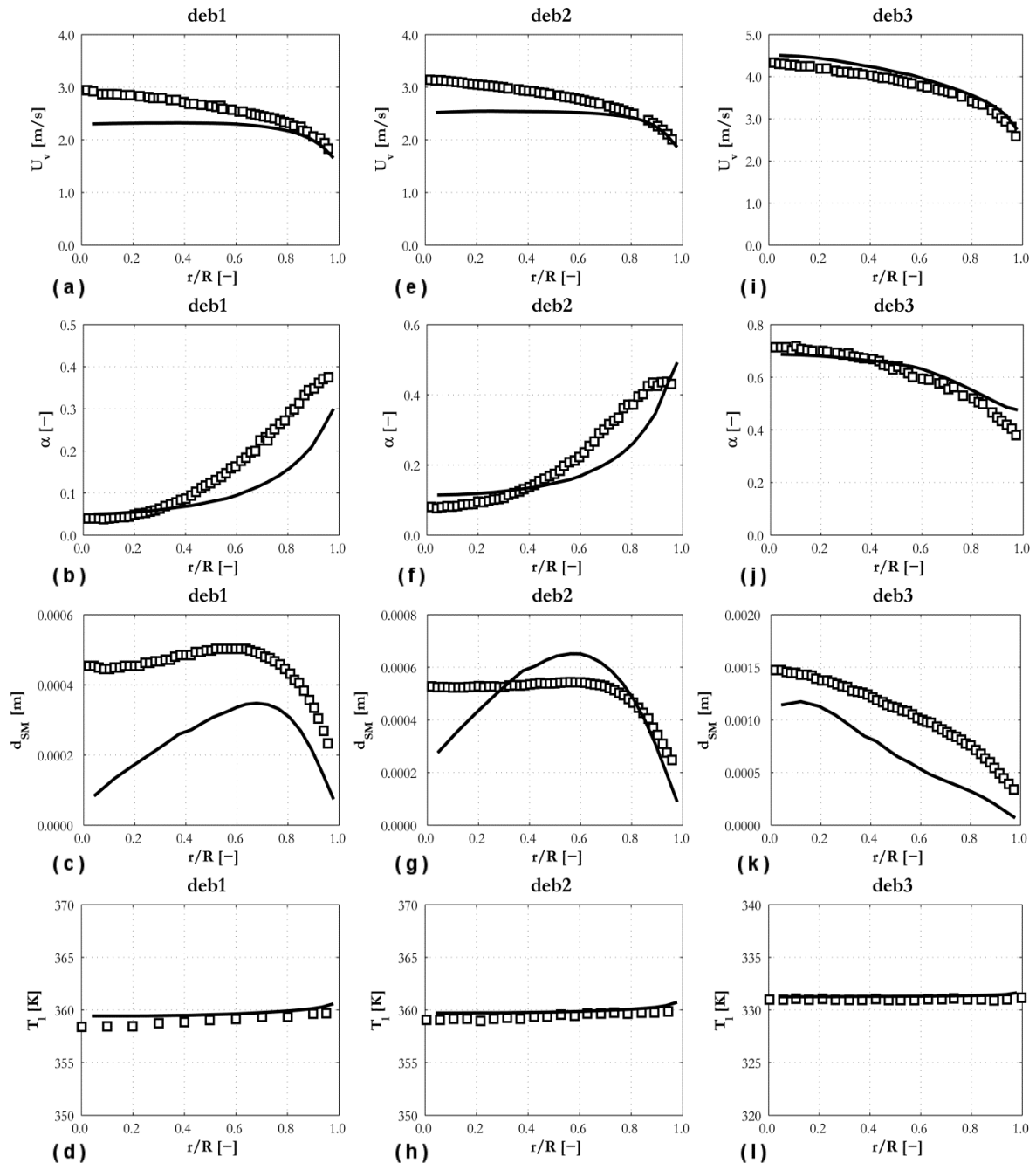
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643 **4.3.5 Turbulence**

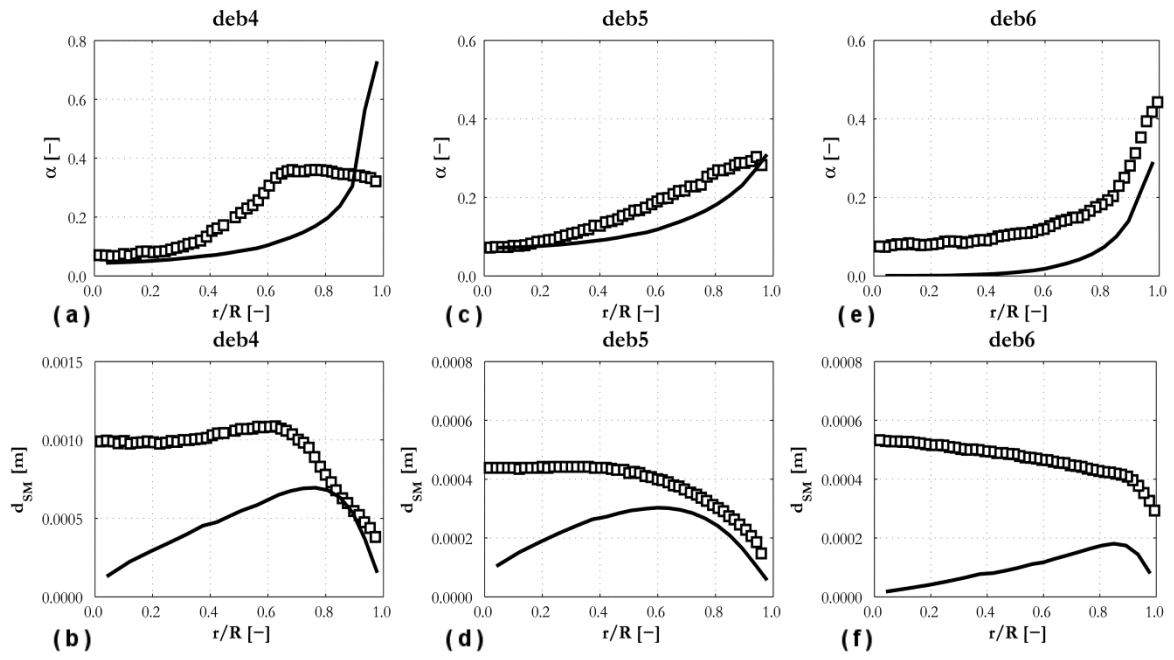
644 Turbulence was only measured by Roy et al. [21] and the streamwise and radial r.m.s. of the
645 liquid velocity fluctuations are shown in Figure 7c, Figure 7g and Figure 7k. Overall,
646 turbulence is well predicted except for the under predicted streamwise r.m.s. in roy1 (Figure
647 7c). Also, the anisotropy of the turbulence field is reasonably well predicted by the Reynolds
648 stress turbulence model.

649 One of the advantages of building such a large database is the opportunity it affords to test
650 any model for all the variables of interest. However, and in view of the present results that

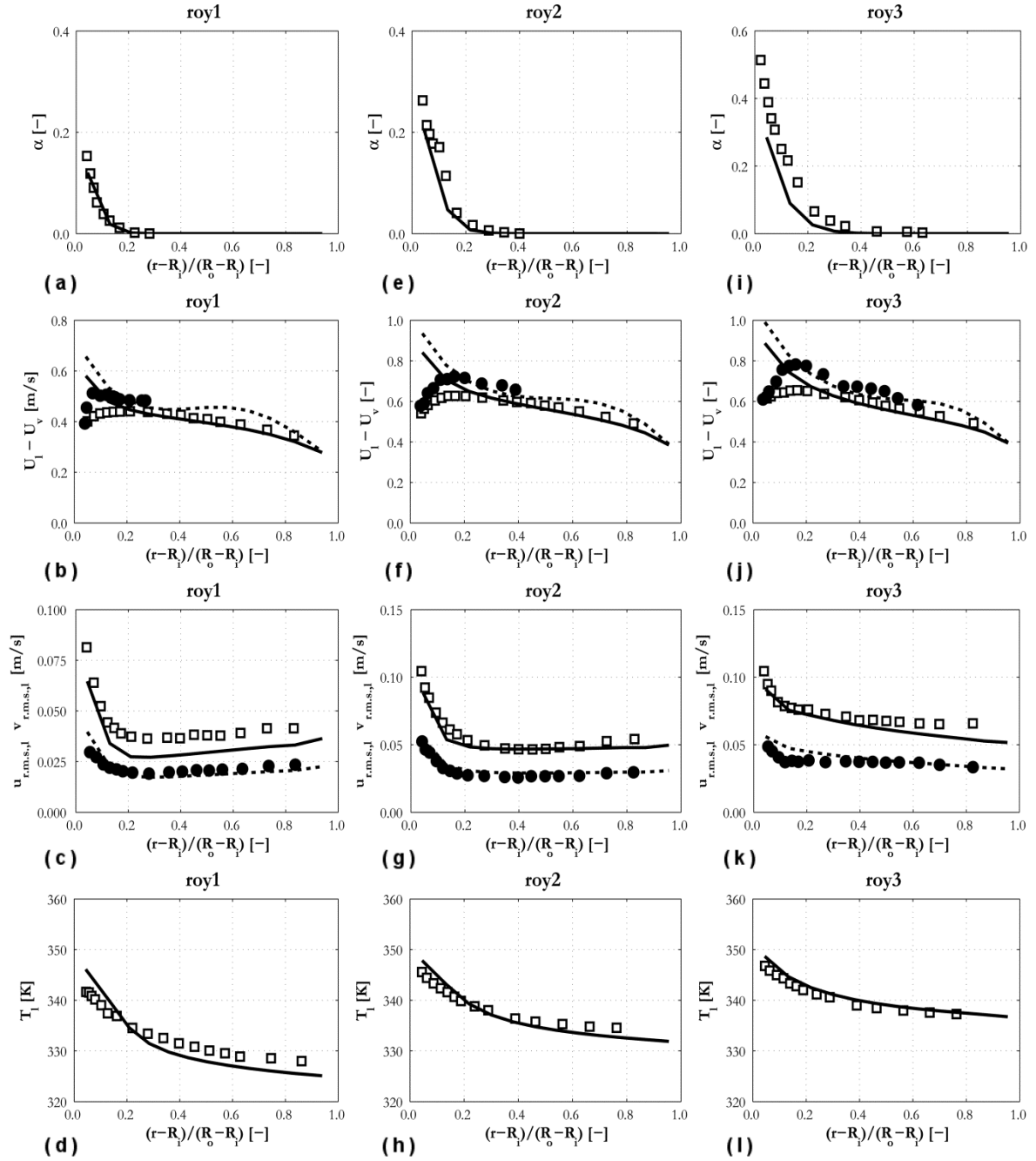
651 show the strengths of the model in some areas but weaknesses in others, measurements of all
 652 the variables of interest in the same experiment are essential to further progress in the
 653 modelling of boiling flows.
 654



655
 656 Figure 5. Average vapour velocity, void fraction, SMD and liquid temperature radial profiles
 657 compared against the DEBORA experiments: (a-d) deb1; (e-h) deb2; (i-l) deb3.
 658

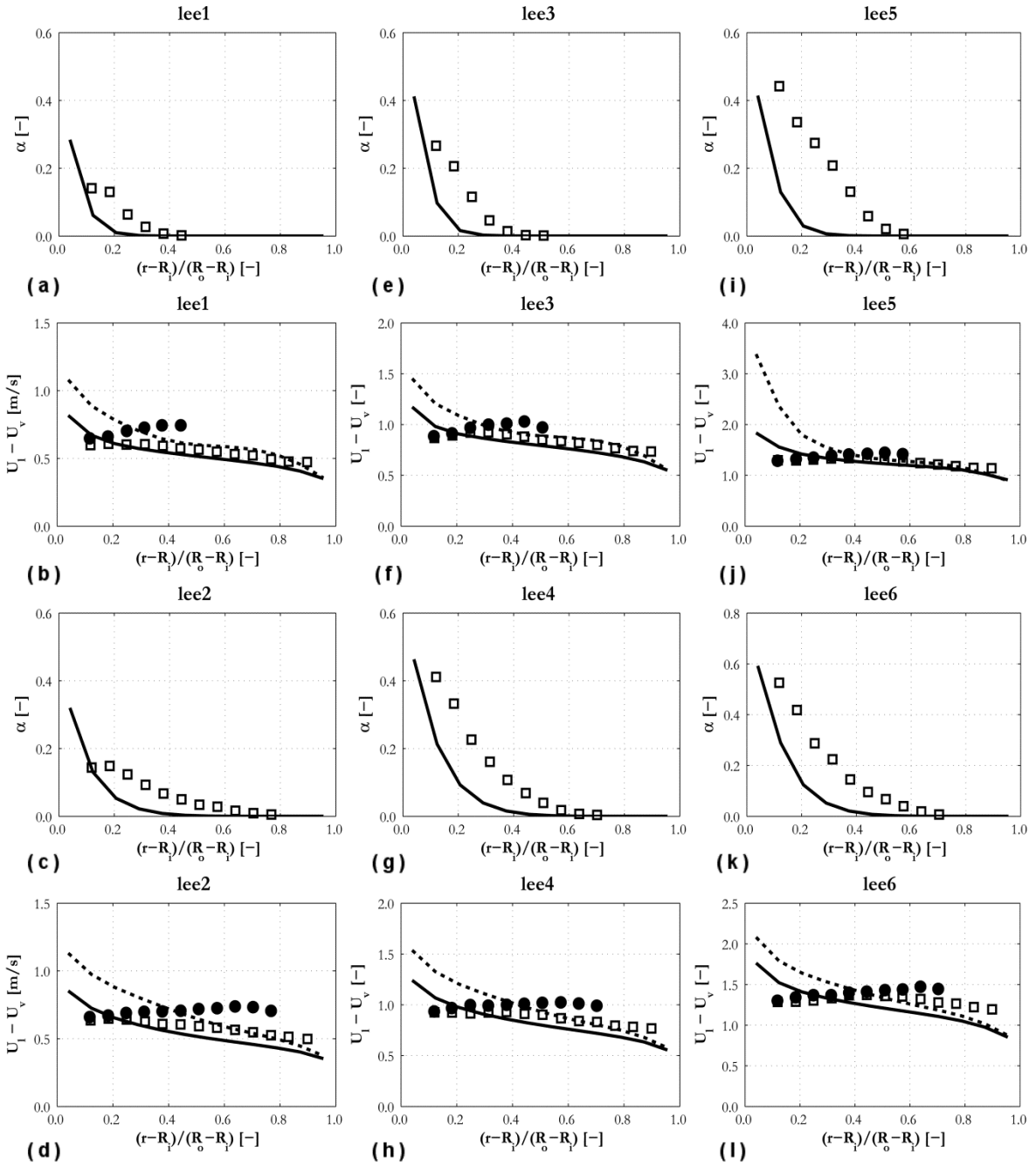


659
 660 Figure 6. Void fraction and SMD radial profiles compared against the DEBORA
 661 experiments: (a-b) deb4; (c-d) deb5; (e-f) deb6.
 662



663
 664 Figure 7. Void fraction, liquid (—,□) and vapour (---,●) average velocity, streamwise (—,□)
 665 and radial (---,●) r.m.s. of liquid velocity fluctuations and liquid temperature radial profiles
 666 compared against Roy et al. [21]: (a-d) roy1; (e-h) roy2; (i-l) roy3.

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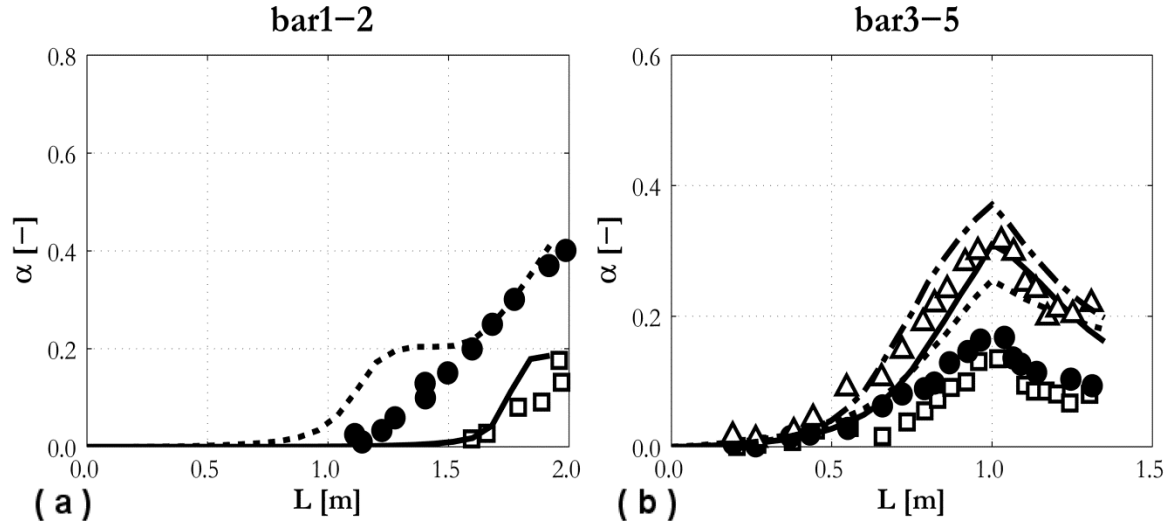
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Figure 8. Void fraction and liquid (—,□) and vapour (---,●) average velocity radial profiles compared against Lee et al. [13]: (a,b) lee1; (c,d) lee2; (e,f) lee3; (g,h) lee4; (i,j) lee5; (k,l) lee6.



676
677 Figure 9. Average void fraction axial development compared against: (a) Bartolomej and
678 Chanturiya [24]; (b) Bartolomej et al. [25]. (a): (—,□) bar1; (---,●) bar2. (b): (—,□) bar3; (---
679 ,●) bar4; (-.-,Δ) bar5.

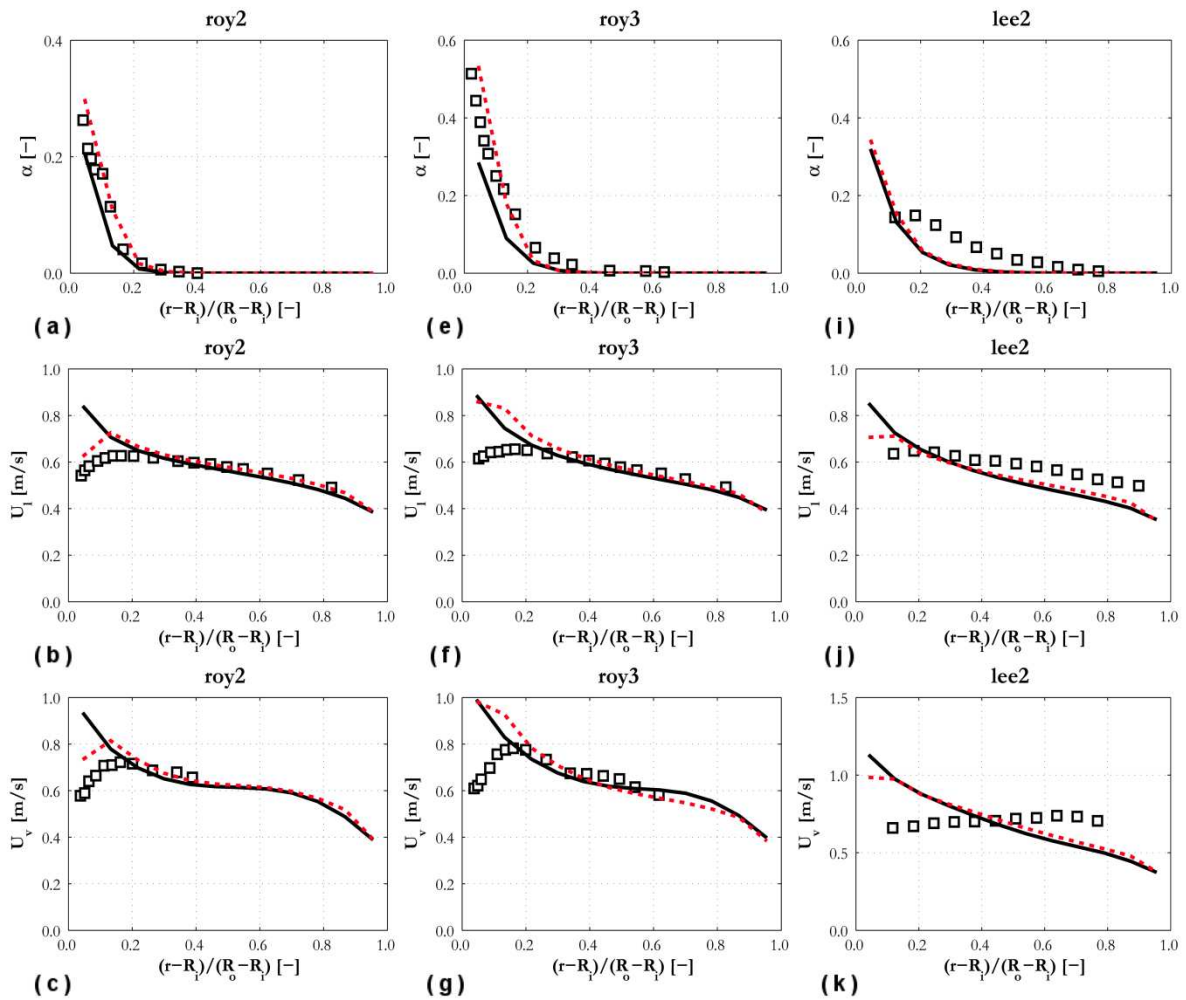
680 681 4.4 Near-wall treatment

682
683 In the previous section, the most significant deviations from experiments were found for the
684 average velocity profiles in the near-wall region of annular channels. In the last
685 computational cell close to the wall, the velocity boundary condition is imposed through the
686 use of wall functions, with the standard single-phase wall function having been used in the
687 simulations. Some authors [8,9,69] have demonstrated how predictions in the near-wall
688 region can be improved with the adoption of a simple wall roughness model, similar to those
689 used in turbulent flows over rough surfaces, but with the equivalent roughness equal to the
690 bubble departure diameter. To the authors' knowledge, such a modification has yet to be
691 tested with an RSM turbulence model. In a first set of simulations with the RSM, it was
692 found difficult to reach convergence and handle the rather high wall roughness values (equal
693 to the bubble departure diameter). Therefore, the wall roughness model was tested using a $k-\varepsilon$
694 formulation. The results are reported in Figure 10 for experiments roy2, roy3 and lee2, and,
695 for the $k-\varepsilon$ model with the standard wall function, these show the same features discussed for
696 the RSM, i.e. liquid and vapour average velocity profiles show the same peak at the wall and
697 rather high values with respect to the experiments.

698 For the lower void fraction cases (roy2 and lee2), agreement for the liquid velocity improves
699 and the profile peaks at a certain distance from the wall with inclusion of the wall roughness
700 model (Figure 10b and Figure 10j). These improvements are limited to the roy2 experiment

701 for the vapour velocity profile (Figure 10c). In the highest void fraction experiment (roy3),
 702 the improvement is also marginal for the liquid velocity (Figure 10f and Figure 10g). In roy2
 703 and roy3, the wall roughness model also produces an increase in the void fraction (Figure 10a
 704 and Figure 10e), although this remains unchanged in lee2 (Figure 10i).
 705 Overall, the introduction of the wall roughness model is seen to improve the predictions,
 706 although the improvements noted are not significant in all cases examined. In addition to
 707 further development of the wall model and its extension for use with RSM, it also seems
 708 necessary, based on the discussion in Section 4.3.4, to better account for the behaviour of
 709 larger bubbles, extending to boiling flows recently developed population balance models that
 710 account for their behaviour separately [10,65].

711



712
 713 Figure 10. Void fraction and average liquid and vapour velocity radial profiles compared
 714 against Roy et al. [21] and Lee et al. [13]: (a-c) roy1; (e-g) roy2; (i-k) roy3. (—) standard
 715 wall function; (---) wall roughness model [8].

716

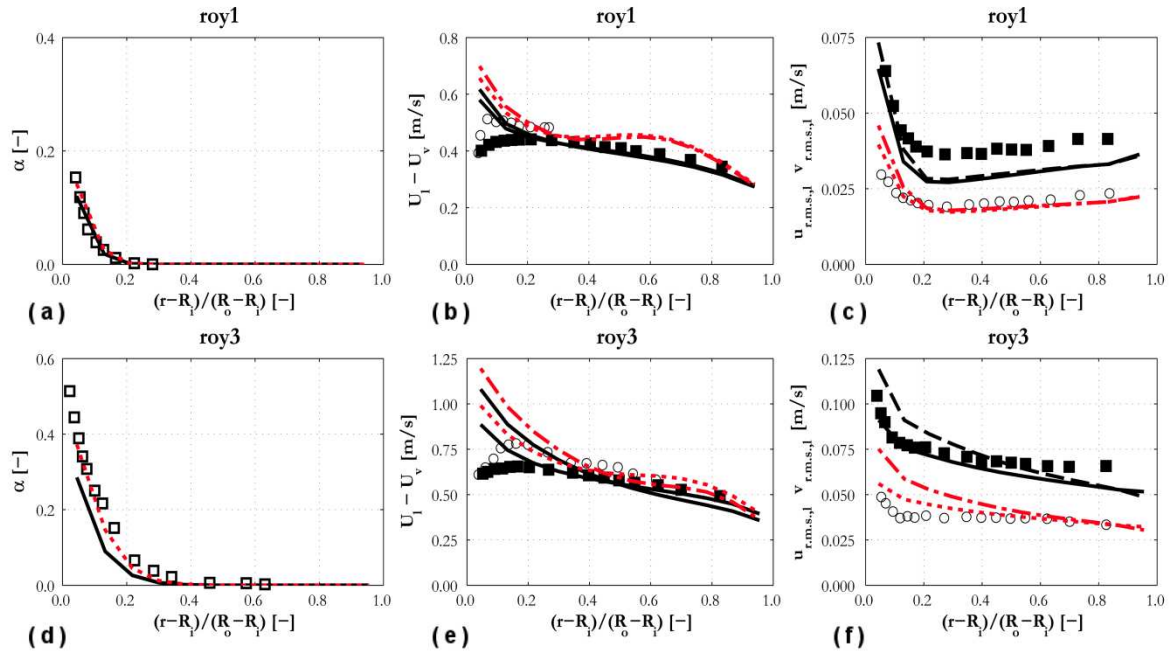
717 **4.5 Bubble-induced turbulence**

718

719 It has been established how, in bubbly flows, the bubbles contribute to the turbulence of the
720 continuous phase and this contribution must be accounted for in the turbulence model
721 [48,54,60]. Many studies have been conducted on the subject, but only a few of them have
722 focused on boiling flows, and, therefore, the impact of the bubble contribution on the
723 turbulence is much more uncertain in these flows. In Section 4.3.5, the bubble-induced
724 contribution was neglected. Nevertheless, turbulence in the continuous phase was well
725 predicted, even if measurements were available only for Roy et al. [21] (Figure 7c, Figure 7g
726 and Figure 7k). This may suggest that bubble-induced turbulence is less important with
727 respect to adiabatic bubbly flows even if it must be noticed that, in Roy et al. [21], the void
728 fraction is very low or zero in the majority of the channel (Figure 7a, Figure 7e and Figure
729 7i). Also, in the regions of high void fraction close to the wall, this influence is further
730 complicated with respect to adiabatic bubbly flows due to the detachment into the bulk fluid
731 of bubbles growing on the heated wall.

732 The roy1 and roy3 calculations were repeated with the bubble-induced turbulence model (Eq.
733 (4) and Eq. (5)) and the results are shown in Figure 11. In roy1, the r.m.s. values are changed
734 only in the region very close to the wall (Figure 11c), where the velocity fluctuations are now
735 overestimated. The same effect is obtained for roy3 and for a larger portion of the pipe
736 section (Figure 11f). Therefore, the model accuracy is generally worsened with inclusion of
737 the bubble-induced turbulence model. Void fraction (Figure 11a and Figure 11d) and average
738 velocity (Figure 11b and Figure 11e) predictions are also increased relative to those without
739 the bubble-induced turbulence contribution. The findings are, however, complicated by the
740 fact that, due to the peak in the velocity profiles, the shear-induced turbulence close to the
741 wall may also be overestimated and this may be the reason for the overestimation of
742 turbulence levels when the bubble-induced contribution is accounted for. More studies are
743 necessary on this subject, but, since bubbles detachment occurs in the first computational cell
744 close to the wall, and in view of the results from the previous section on the wall treatment, it
745 is suggested that the problem needs to be approached globally, addressing jointly in the same
746 model the velocity boundary condition and the generation of turbulence close to the wall, as
747 well as the contribution from the bubbles in this region.

748



749

750 Figure 11 Void fraction, liquid (\square ,—,—) and vapour (\circ ,---,---) average velocity and
 751 streamwise (\square ,—,—) and radial (\circ ,---,---) r.m.s. of the liquid velocity fluctuations radial
 752 profiles compared against Roy et al. [21]: (a-c) roy1; (d-f) roy3. (—,---) without bubble
 753 induced turbulence model; (---,---) with bubble induced turbulence model.

754

755 5 Conclusions

756

757 An Eulerian-Eulerian two-fluid CFD model, including a Reynolds stress turbulence model,
 758 the method of moments-based S_j population balance approach and a boiling model derived
 759 from the RPI heat flux partitioning approach, was used to predict a large database of
 760 subcooled boiling flows. The database includes 20 experiments of subcooled boiling flows of
 761 water and refrigerants in vertical pipes and annular channels, and covers a wide range of
 762 conditions.

763

764 Overall, the model confirms the potential of CFD to provide detailed predictions of boiling
 765 flows and rather good agreement with data was found in some areas, but others still require
 766 significant improvements in model accuracy. At the present time, the general applicability of
 767 the model is not entirely satisfactory. Even if built in a mechanistic fashion, numerous
 768 empirical closure relations are required, not only for wall boiling, but also for the population
 769 balance and turbulence models. This clearly limits the overall model's general applicability
 770 and, therefore, the development of more mechanistic closures is highly desirable. A good
 771 example is provided by the bubble departure diameter that cannot be predicted with accuracy
 over extended ranges of conditions by the presently available correlations. The development

772 of physically-based, more accurate closure models is challenging and may only be achieved
773 with an increase in our knowledge of mechanisms that are as yet not completely understood,
774 such as the growth and departure of bubbles, but also their breakup and coalescence and the
775 interaction of turbulence with bubbles near the wall, amongst others.

776 The results show how studies such as the one described, which focused on a large database,
777 can profitably be used to integrate detailed analyses based on more limited amounts of data.
778 In the latter, major developments of specific sub-models can be derived and tested, but these
779 developments can only be accepted if they improve the general accuracy of models when
780 tested against large sets of data. The disparity observed between individual experiments
781 suggests that it is risky to judge the accuracy of any CFD model on the basis of a limited
782 number of comparisons with data.

783 Quantitatively, the predictive accuracy is satisfactory for the void fraction, except for a
784 limited number of cases, with the turbulence and liquid temperature fields also well
785 predicted. In contrast, the average bubble diameter, quantified by the SMD, tends to be
786 underestimated, sometimes significantly, in particular near the axis of the flows, with velocity
787 profiles also over predicted near the heated wall of annular channels, where they exhibit a
788 peak that is instead found away from the wall in the experiments.

789 Despite the inaccuracy of some predictions, the satisfactory results achieved in some areas
790 encourage further research:

- 791 • No correlation for the bubble departure diameter was found appropriate for the entire
792 database and the under prediction of the departure diameter was identified as a
793 possible source of error in the average bubble diameter predictions. The use of more
794 mechanistic formulations, already adopted by a limited number of researchers,
795 represents a way forward in this regard.
- 796 • Modelling of bubble break-up and coalescence needs to be improved, with related
797 improvements in population balance modelling also required. More specifically, the
798 ability to account for larger bubbles moving towards the flow centre, already available
799 for adiabatic flows, may improve the prediction of velocity profiles in both pipes and
800 channels.
- 801 • Velocity predictions near the wall were improved using a wall roughness model, but
802 further development is required, in particular in the context of RSM.
- 803 • Bubble-induced turbulence was demonstrated to be less relevant with respect to
804 adiabatic flows and the use of a specific model provided inconsistent results. A more

805 advanced modelling approach seems necessary near the wall, but it should be
806 addressed together with the wall treatment.

807

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809

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813

814 **Nomenclature**

815 A_b fraction of the wall affected by the evaporation process [m^{-1}]

816 a_i interfacial area concentration [$m^2 m^{-3}$]

817 C_D drag coefficient [-]

818 C_p specific thermal capacity at constant pressure [$J kg^{-1} K^{-1}$]

819 D diameter [m]

820 d_B bubble diameter [m]

821 d_{crit} critical bubble diameter [m]

822 d_{SM} Sauter mean diameter [m]

823 d_w bubble departure diameter [m]

824 Eo bubble Eotvos number $Eo = g (\rho_l - \rho_v) d_B^2 / \sigma$ [-]

825 F_d drag force [$N m^{-3}$]

826 F_{TD} turbulent dispersion force [$N m^{-3}$]

827 f frequency of bubble departure [s^{-1}]

828 G mass flux [$kg m^{-2}s^{-1}$]

829 g gravitational acceleration [$m s^{-2}$]

830 h_q quenching heat transfer coefficient [$W m^{-3}K^{-1}$]

831 i_{lv} latent heat of vaporization [$J kg^{-1}$]

832 K_{br} break-up rate [s^{-1}]

833 $K_{cl}^{d,d'}$ coalescence rate [s^{-1}]

834 K_{dry} fraction of the heated wall in contact with the vapour phase [-]

835 k turbulence kinetic energy [m^2s^{-2}]

836 L pipe/channel length [m]

837 M_γ γ^{th} moment of the bubble diameter distribution [m^γ]

838 m_{lv} interphase mass transfer [$kg m^{-3}s^{-1}$]

839 N bubble generation rate per unit volume [$bubbles m^{-3}s^{-1}$]

840	N_f	number of daughter bubbles [-]
841	n	bubble number density [bubbles m ⁻³]
842	n'	nucleation site density [m ⁻²]
843	$P(d_B)$	bubble diameter probability distribution [-]
844	Pr	Prandtl number $Pr = C_p \mu / k$ [-]
845	p	pressure [Pa]
846	p_r	reduced pressure p/p_{crit} [-]
847	Q_{ev}	evaporative volumetric heat flux [W m ⁻³]
848	Q_l	liquid phase convective volumetric heat flux [W m ⁻³]
849	Q_q	quenching volumetric heat flux [W m ⁻³]
850	Q_v	vapour phase convective volumetric heat flux [W m ⁻³]
851	Q_w	total wall volumetric heat flux [W m ⁻³]
852	q''	heat flux [W m ⁻² K ⁻¹]
853	R	radius [m]
854	R_g	gas constant [J mol ⁻¹ K ⁻¹]
855	R_{ij}	Reynolds stress [m ² s ⁻²]
856	r	radial coordinate [m]
857	Re	bubble Reynolds number $Re = \rho_l U_r d_B / \mu_l$ [-]
858	S_{br}	source of S_γ due to bubble break-up [m ^{γ} m ⁻³ s ⁻¹]
859	S_{cl}	source of S_γ due to bubble coalescence [m ^{γ} m ⁻³ s ⁻¹]
860	S_m	source of S_γ due to boiling and evaporation [m ^{γ} m ⁻³ s ⁻¹]
861	S_k^{BI}	bubble-induced turbulence kinetic energy source [kg m s ⁻³]
862	S_ϵ^{BI}	bubble-induced turbulence energy dissipation rate source [kg m s ⁻⁴]
863	S_γ	density of the γ^{th} moment of the bubble diameter distribution [m ^{γ} m ⁻³]
864	ΔS_γ^{br}	change in S_γ due to a single break-up event [m ^{γ}]
865	$\Delta S_{\gamma,cl}^{d,d'}$	change in S_γ due to a single coalescence event [m ^{γ}]
866	T	temperature [°C]
867	T^+	dimensionless temperature [-]
868	t	time [s]
869	t_w	waiting time for bubble departure [s]
870	U	velocity [m s ⁻¹]
871	$u_{r.m.s.}$	streamwise r.m.s. of the velocity fluctuations [m s ⁻¹]
872	$v_{r.m.s.}$	radial r.m.s. of the velocity fluctuations [m s ⁻¹]

873	u_τ	shear velocity [m s^{-1}]
874	We	Weber number $We = \rho_l u d_B / \sigma$ [-]
875	We_{crit}	critical Weber number [-]
876	x	spatial coordinate [m]
877	y^+	dimensionless wall distance [-]
878	α	void fraction [-]
879	ε	turbulence energy dissipation rate [m^2s^{-3}]
880	θ	contact angle [rad]
881	λ	thermal conductivity [$\text{W m}^{-1}\text{K}^{-1}$]
882	μ	viscosity [Pa s]
883	ν_t	turbulent kinematic viscosity [m^2s^{-1}]
884	ρ	density [kg m^{-3}]
885	σ	surface tension [N m^{-1}]
886	τ_{BI}	bubble-induced turbulence timescale [s]
887	τ_{br}	break-up timescale [s]

888

889 ***Subscripts***

890	c	continuous phase
891	d	dispersed phase
892	i	inner
893	in	inlet
894	l	liquid
895	o	outer
896	r	relative
897	sat	saturation
898	v	vapour
899	w	wall

900

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