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A review on numerical modelling of flashing flow with application to nuclear safety analysis

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Abstract

The flashing flow is an relevant multiphase phenomenon in many technical applications including nuclear safety analysis, which has been the subject of intense research. Numerical studies have evolved from one-dimensional to multidimensional. A variety of methods have been proposed, while a broad consensus was not exiting. The present work aims to present an overview of available models as well their assumptions and limitations by conducting a literature survey. The final focus was put on recent computational fluid dynamics simulations. Some consensus on modelling interfacial slip, phase change mechanism and bubble size is identified. Since flashing scenarios often accompanying with high void fraction and broad bubble size range, a poly-disperse two-fluid model is recommended. Thermal phase change model is superior to pressure phase change, relaxation and equilibrium models for practical flashing problems. Major challenges include improving closure models for interphase transfer, bubble dynamics processes, interfacial area as well two-phase turbulence. For this purpose, high-resolution high quality experimental data are important, which are lacking in many cases. Considering that heterogeneous gas structures often exist in flashing flows, multi-field approaches able to handle different shapes of gas-liquid interface are recommended.

Keywords: computational fluid dynamics, flashing flow, nuclear safety analysis, numerical modelling, literature review

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1 1. Flashing phenomenon and its relevance to nuclear safety

Production of steam from water boiling is a familiar process under normal operation of light water nuclear reactors, for example, in the core of Boiling Water Reactors (BWRs) and in the Steam Generator (SG) of the Pressurized Water Reactors (PWRs). In these normal situations, water is heated to sat-5 uration temperature by a hot structure or heat source, e.g. fuel rods in the core or U-tubes in the SG, and steam as energy carrier drives the turbine generators to produce electricity. On the other hand, phase change from liquid to 8 vapor can be triggered by depressurization under nearly adiabatic conditions. Pressure drop may occur in pipes with varying cross section and enhanced el-10 evation, in relief values, breaks or other types of mechanical failures[1]. The 11 pressure-driven phase change can be considered as a spectrum of phase change 12 phenomena with cavitation at the cold end and flashing at the hot end [2, 3]. In 13 the case of hot liquids, the temperature of liquid remains almost constant till the 14 phase change starts, but the saturation temperature drops with the pressure. 15 As the pressure of the liquid reaches the saturation pressure corresponding to 16 its temperature, boiling i.e. formation of vapour bubbles takes place as a result 17 of interfacial heat transfer, but sometimes the pressure has to drop below the 18 saturation point [2]. The bubble growth and vapor generation is predominantly 19 controlled by the heat transfer rate at the liquid-vapor interface. The difference 20 between the saturation pressure and the pressure at boiling inception is often 21 referred to as pressure undershoot characterizing the maximal non-equilibrium 22 between the liquid and vapor phases [4]. Its value depends on the initial tem-23 perature of liquid, depressurization rate, liquid and vapour properties as well 24 nucleation sites available in the system. The thermally-controlled vaporization 25 process under depressurization is commonly referred to as flashing in the com-26 munity of nuclear engineering, but more often as flash evaporation in the field 27 of desalination [5–8] and flash boiling in spray atomization [9–12]. The flashing 28 phenomenon has received great interest from various branches, and a review on 29

its application and consequence as well existing experimental, theoretical and 30 numerical studies is given by [13]. Although many industrial processes ben-31 efit from the flashing phenomenon, for example, steam and spray generation 32 [14, 15], absorption and oxidation [16, 17] as well as desalination for gaining 33 drinking water [18–20], the fast phase change process may have a significant 34 impact on the safety and performance of many devices and systems. Concern-35 ing nuclear safety analysis, flashing behavior is of key importance in terms of 36 determining the reduction rate of reactor coolant inventory and affecting core 37 thermal-hydraulics during the loss of coolant accident (LOCA), and inducing 38 flow instabilities in passive safety systems driven by natural circulation. 39

40 1.1. Flashing-related topics under LOCA conditions

• Critical flow problem: In the frame of nuclear safety analyses numer-41 ous researchers have investigated steady-state flashing flows through pipes, 42 nozzles, orifices and other restrictions in relation with critical flow problem 43 [21, 22]. In such flows vaporization develops under a constant pressure dif-44 ference between the inlet and exit of the pipe. As the exit pressure drops 45 below a critical value, the flow rate doesn't increase anymore, which is re-46 ferred to as critical (or chocked) flow. A large body of literature on both 47 experimental and numerical studies arose in the period from late 1960s to 48 early 2000s, e.g. [23-30] among many others. Most of the efforts are driven 49 by the need of predicting maximal flow rates under critical conditions, 50 since it determines the rate at which coolant inventory leaves the reactor 51 cooling system in LOCAs. Among others the BNL (Brookhaven National 52 Laboratory) experiments on flashing flow in a converging-diverging circu-53 lar nozzle [26] have been analyzed in many numerical works, e.g. [31–41]. 54

Pipe blowdown transient: There have been also many experimental and theoretical works on transient two-phase flashing flows under pipe blowdown conditions. The major concern here is the early-stage response of initially subcooled but hot liquid in a pipe or vessel during sudden de pressurization, including the change of fluid temperature and pressure as

well as the inception of flashing and void development. The information 60 is of importance for analyzing the system behaviour and checking over 61 the action of safety and protection systems during the accident. Edwards 62 and O'brien [42] performed transient blowdown experiment using a 4.09 m63 long 0.073 m diameter pipe. The horizontal pipe was filled with pressur-64 ized heated water, a glass disk at one end was ruptured to initiate the 65 blowdown. The measurements of pressure at several positions as well as 66 void fraction have been used for model validation in a number of numeri-67 cal works such as [43–45]. Takeda and Toda [46] investigated the pressure 68 behavior in a vertical pipe ruptured at the top end with an initial temper-69 ature gradient increasing from bottom to top. The case was analyzed by 70 Lafferty et al. [47] and Costa et al. [48] with the RELAP5 and WAHA code, 71 respectively. Similar blowdown experiments were conducted by Lienhard 72 et al. [49], Bartak [50] and others. Instead of analyzing the transient 73 pressure behavior in the tube, the objective of these studies was the study 74 of the nucleation delay phenomenon. Semi-empirical correlations based 75 on the classical nucleation theory and experimental data were derived for 76 determining the pressure undershoot. 77

• Lower plenum flashing: Although the study of pipe critical flow and 78 blowdown phenomena is a contributing part of the LOCA analysis, the 79 fluid behavior and steam generation in the pressure vessel is as well of great 80 interest in the nuclear safety analysis. It affects directly the core cooling 81 and occurrence of core meltdown. As the downcomer level falls, the ini-82 tially subcooled lower plenum may exceed saturated conditions and flash, 83 resulting in a surge of two-phase flow upwards through the core to the 84 upper plenum. This may reduce the liquid inventory in the lower plenum 85 and downcomer because of vaporization and entrainment, and may also 86 reduce the reflood driving head and prevent the injected cooling water 87 from entering the downcomer. Nevertheless, the liquid entrained in the 88 steam flowing toward the upper part of the vessel may often give a signifi-89

cant contribution to the cooling of uncovered fuel rods, both in PWR and 90 BWR systems [51, 52]. Transient two-phase flashing flow in the core or 91 large pipes relative to the phenomenon of counter-current flow limitation 92 (CCFL) is investigated insufficiently, due to the complexity of the incident. 93 Phenomenologically, the flashing effects observed in the lower plenum can 94 also be encountered in control rod guide tubes. Because of different ge-95 ometry and initial liquid subcooling, the flashing intensity is lower and 96 thus less important than the previous one as far as nuclear reactor safety 97 is considered. Nonetheless, it may affect the core thermal-hydraulic be-98 haviour in a later stage of LOCA transients [51]. In comparison to pipe 99 critical or blowdown flows mentioned above, investigation on the flashing 100 process occurring inside the vessel is challenging due to the large geometry 101 size as well as complex internals. A limited number of studies were per-102 formed in this area, and a few large-scale experiments on blowdown effects 103 in the pressure vessels are available, e.g. [53–55]. Recently, Wang et al. 104 [56] studied the two-phase flow instability in a PWR-type small modular 105 reactor under LOCA conditions. The temperature and void fraction tran-106 sients were measured at four ports in the core and riser, and the pressure 107 drop between these ports as well as between the top and the bottom of 108 the containment was measured through differential pressure drop trans-109 ducers. Ylönen [57] reviewed existing experiments on large-break LOCA, 110 and concluded that for the purpose of CFD code validation, suitable data 111 such as pressure and void fraction at both axial and radial positions are 112 needed. 113

• SG tube rupture flashing: In a PWR steam generator (SG) tubes constitute a large fraction of the reactor primary coolant loop pressure boundary. The SG tubes play an important safety role. Any leakage resulting from SG tube rupture (SGTR) will allow radiation to escape into the non-radioactive side of the plant and likely to environment, the function containment being bypassed [58]. Although the core melt fre-

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quency resulting from SGTR is low relative to other severe accidents, it 120 is a major accident in the field of nuclear safety considering its direct im-121 pact on the environment. Coolant flow rate through the break is a key in 122 the analysis of SGTR. Due to high pressure drop through the break, the 123 coolant flashes rapidly and the flow becomes chocked or critical. As intro-124 duced above the critical flow problem has been a subject of intense study 125 both experimentally and theoretically. However, the research in the past 126 mostly focused on blowdown from vessels, large pipes or short nozzles, 127 while SGTR presents a particular class of small-break LOCAs (SBLO-128 CAs). The width of the crack is in the micrometer range and the length 129 of flow path approximates the thickness of SG tube walls ($\sim 1mm$) [59]. 130 Assessment and extension of numerical models is necessary. The over-131 all system performance of a light water PWR during SGTR events with 132 different number of ruptured tubes and with/without ECCS (Emergency 133 Core Cooling System) was tested in many institutions [60–63]. 134

135 1.2. Flashing-induced instability (FII)

Passive systems utilizing natural circulation have advantages over active 136 ones, and are frequently adopted in new generation reactors [64]. The passive 137 containment cooling system (PCCS) has been developed as an advanced safety 138 feature, for example, in AP1000 [65], ESBWR[66], iPOWER [67], VVER-1200 139 [68], KERENATM [69], and the Hualong pressurized reactor 1000 (HPR1000) 140 [70]. A major disadvantage of the passive systems is the low driving force, which 141 can lead to instability and safety problems. Due to hydrostatic pressure drop 142 in the riser of natural circulation loop, steam generation by flashing can take 143 place. As the steam bubbles condense in cold parts of the loop, oscillation of 144 flow rate, temperature and pressure can be observed, which is referred to as 145 Flashing-induced instability (FII). The FII phenomenon was first observed by 146 Wissler et al. [71] as they conducted experiments on an open natural circu-147 lation test loop. Since then, many researchers performed experimental studies 148 on the phenomenon, and a majority part focused on the instability problem 149

in BWR during start-up, e.g. [72–75]. At the start-up condition, the coolant 150 may not reach saturation temperature in the core, where it is heated up, and 151 remain single-phase due to low power. However, because of considerable de-152 crease in coolant saturation temperature along the flow path, flashing can occur 153 in the adiabatic section above the core, and lead to self-sustained flow oscil-154 lation in the loop. A flashing-driven passive moderator cooling system was 155 developed at AECL for CANDU reactors. It was shown that the concept was 156 feasible at normal operating power, but caused flow instabilities at low power 157 [76, 77]. Similar phenomena were observed in the PCCS systems mentioned 158 above. Recently, Cloppenborg et al. [78] investigated two-phase phenomena in 159 the KERENATM-CCC (containment cooling condenser) natural circulation sys-160 tem on the GENEVA test circuit. The riser section is two times longer (~ 9m) in 161 comparison to other natural-circulation systems such as CIRCUS [72], equipped 162 with high time and spatial resolution instrumentation for local void fraction and 163 temperature distribution. Since the late 1980s, many researchers have analyzed 164 the FII using numerical methods, and various analysis codes were adopted such 165 as TRACG [79], FLOCAL [80], RELAP5 [81, 82] and MARS [64, 83]. Lim et 166 al.[64] attempted to develop stability maps for FII using the MARS code. Due to 167 high-frequency transients and complex two-phase processes, high-fidelity mod-168 elling of FII represents still great challenge and difficulty. 169

¹⁷⁰ 2. Widely-used numerical models for flashing flows

As aforementioned, a large body of literature exists on the numerical study 171 of various flashing scenarios conducted with application to nuclear safety anal-172 ysis. The simulations progress from one-dimensional to three-dimensional. The 173 models range from simple empirical to mechanistic ones with different levels 174 of sophistication. Concerning whether non-homogeneous non-equilibrium ef-175 fects are considered, they fall into four main categories (a) homogeneous equi-176 librium model (HEM), (b) non-homogeneous equilibrium model (NHEM), (c) 177 homogeneous non-equilibrium model (HNEM) and (d) non-homogeneous non-178

Models	Features	Subcategory	Reference examples
HEM	equal velocity		[84 80]
	equal temperature		[04-09]
	unequal velocity	slip ratio model	[27, 28, 84, 90]
NHEM	equal temperature	drift-flux model	[91, 92]
		two-fluid model	[21, 93, 94]
HNEM	equal velocity	empirical model	[28,42,95100]
	unequal temperature	relaxation model	[101 - 107]
		delayed equilibrium model	[108, 109]
		physically-based model	[31, 43, 110 - 112]
NHNEM	unequal velocity	drift-flux model	[30, 32, 102, 113]
	unequal temperature	two-fluid model	[81, 114, 115]

Table 1: Overview of numerical models for flashing flows

equilibrium model (NHNEM). The term "homogeneous" here means equal velocities while "equilibrium" denotes equal temperatures of the liquid and vapor phases. The models in each category differ further in their treatment of the mechanical and thermal non-equilibrium and the applied constitutive models, see Table 1. A brief introduction of these models, and a review on representative one-dimensional numerical works are provided in this section, while threedimensional simulations are discussed subsequently.

186 2.1. The HEM model

As the name suggests, the HEM model simplifies the two-phase flow to a pseudo or an equivalent single-phase one flowing with an average velocity and possessing mean thermodynamic properties, which are obtained by interpolating between the saturated liquid and vapour ones using the equilibrium quality. In order to use well-established single-phase theories, the HEM model was very often used for LOCA analysis around 1950s, for example, available in early ver-

sions of the system code RELAP. Among others Leung [116] presented a critical 193 flow model on the basis of HEM assumptions. It works well for long pipes for 194 example with a length exceeding 3.0 inches [84], where the time is sufficient 195 for equilibration between the phases. Many works [84-87] discuss the difference 196 between measured and predicted critical flow rates for short pipes, in which 197 there is insufficient time for the two-phase mixture to proceed to equilibrium. 198 The flow rates predicted by the HEM model are considerably less than those ob-199 tained experimentally. Deligiannis and Cleaver [112] found that the HEM model 200 is incapable of predicting the earliest stage of a rapid depressurization, where 201 the effect of nucleation and thermal non-equilibrium is of prime importance. 202 Inada [88] and Van Bragt et al. [89] investigated flashing effects and instability 203 mechanisms in a natural circulation BWR using the HEM model. Concerning 204 the flow instability Hu et al. [117] and Podowski [118] reported that the HEM 205 predictions are conservative in comparison with a slip or two-fluid model, be-206 cause the HEM void fraction is higher. According to [29] in the initial stage of 207 steady-state flashing, when bubbles are small and finely dispersed in the liquid, 208 an assumption of hydrodynamic momentum equilibrium is applicable, however, 209 thermal non-equilibrium has to be considered since the interfacial area available 210 for heat transfer is very limited. As the bubbles grow and void fraction exceeds 211 a value of 0.3, thermal equilibrium may be assumed but slip between the phases 212 becomes important and ignoring it will cause inaccuracies. 213

214 2.2. NHEM models

Attou et al. [93] studied the effect of interfacial slip on bubbly flow through 215 a sudden enlargement by analyzing two extreme conditions with maximum or 216 negligible momentum transfer between the two phases, respectively. The for-217 mer assumption is equivalent to HEM, while the latter was referred to as a 218 momentum frozen model (MFM). It was found that in HEM, due to complete 219 momentum transfer between the phases, the lower inertia of the gas causes the 220 liquid to decelerate faster than in reality, leading to a higher pressure recovery 221 than predicted in experiments. Consequently, the MFM causes the liquid to 222

decelerate slower and hence the pressure recovery predicted is lower than in 223 experiments. Addressing the finite rate of interphase transfers is of importance 224 in analyzing flashing flows especially at the later stage [29]. Most earlier ef-225 forts have been devoted to developing empirical or theoretical correlations for 226 the velocity (or slip) ratio. The theoretical models for critical flow presented 227 in [27, 28, 84, 90] for long tubes are based on the thermodynamic equilibrium 228 assumption but relax the requirement of equal phase velocities by introducing 229 a slip ratio. The next level of complexity is to use the drift-flux model to char-230 acterize the effect of the relative motion, which evaluates the void distribution 231 parameter and the vapor drift velocity pure empirically. Hu et al. [91] investi-232 gated the FII during a BWR reactor start-up using a NHEM model. The vapor 233 generation rate was derived from the mixture energy conservation equation, 234 while the nonhomogeneous velocities of the liquid and vapor was considered us-235 ing the drift-flux approach. A similar equilibrium approach was used in [92] for 236 the linear stability analysis of a boiling natural circulation loop. On the other 237 hand, Wallis [21] and Bouré [94] disadvised the use of drif-flux models. They 238 warned that the relative motion in a rapidly accelerating/decelerating flow with 239 changing void fraction as well flow pattern is determined by a quite different set 240 of terms from which the derivation of drift-flux correlations is based on. It is 241 important to take into account the mechanical interaction between the phases 242 using a separated flow model or two-fluid model when the flashing flow has to 243 be modelled [93]. 244

245 2.3. HNEM models

Similar to homogeneity of phase velocities, the validity of assumption about thermal equilibrium is limited. According to Donwar-Zapolski et al. [119], the most important feature of flashing flows is the thermal non-equilibrium effects caused by nucleation delay and limited rate of vapor generation. Flashing starts with some delay until the pressure drops below the saturation line, and the real quality pattern differs essentially from the equilibrium one. This greatly influences the void fraction as well as the pressure and velocity distribution along the flow. Kato et al. [120] presented an equation which gave the relative importance of inertial and thermal effects controlling bubble growth in superheated liquid. It was shown that the model has to capture the non-equilibrium nature of the flow in order to simulate flash boiling accurately [121]. The methods describing thermal non-equilibrium fall in four categories:

• Empirical models: The HEM model is known to over-predict the vapor 258 generation rate and thus under-predict the flow rate in the critical flow. 259 Henry and his co-workers [28] intended to consider the non-equilibrium 260 effect by introducing a correction factor, which allows only a fraction of 261 the equilibrium vapor generation to occur. The empirical factor was de-262 rived based on the deviation between the measured flow rate and the HEM 263 prediction, and its expression largely depends on the pipe length to diam-264 eter ratio. For a slip ratio value of unity the authors presented a simple 265 correlation being a function of equilibrium quality only. It assumes that if 266 the quality exceeds 0.05 thermal equilibrium is achieved. For low qualities 267 the non-equilibrium factor was set to 20 times the equilibrium quality, i.e. 268 $N = 20x_{eq}$. The actual flow rate was estimated as $G_{HEM}/N^{1/2}$, where 269 G_{HEM} is the flow rate obtained from the HEM model. In their homo-270 geneous model assuming equal phase velocities, Simpson and Silver [95] 271 and Edwards [42] introduced two empirical coefficients to account for the 272 non-equilibrium nucleation process. One is the time-delay for bubble nu-273 cleation, and the other is the number concentration of bubble nuclei. For 274 sake of simplicity Lackmé [96] assumed that evaporation should start if the 275 pressure falls about 5% below the saturation pressure. To determine the 276 nucleation delay more reliably, many experimental and theoretical works 277 on the determination of pressure-undershoot have been carried out, e.g. 278 [4, 50, 97, 98] among others. Based on the classical homogeneous nu-279 cleation theory and measurement of pressure-undershoot, semi-empirical 280 correlations were proposed, which have been frequently used in the one-281 dimensional analysis of flashing critical flows such as [99, 100]. A brief 282

summary of such models as well their applications was given in [2, 122].

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• Relaxation models: The basic idea of the relaxation model is that the 284 actual quality x is lower than the equilibrium one x_e . It increases propor-285 tionally to the difference between them during the flashing process. The 286 relaxation model for LOCA analysis was first discussed in [101, 102], where 287 the vapor generation rate is correlated with $x_e - x$. Bilicki and Kestin [103] 288 proposed the homogeneous relaxation model (HRM) by adding a rate 289 equation to the HEM equations. It describes the rate of the actual quality 290 x approaching its local equilibrium value. The necessary coefficient is the 291 relaxation time, which is a function of system pressure, mixture enthalpy 292 and actual quality. Downar-Zapolski et al. [119] derived a correlation for 293 the relaxation time basing on the "Super Moby Dick" experiments on criti-294 cal flow rates [23]. It is a monotonically decreasing function of void fraction 295 and the non-dimensional pressure difference $(p_{sat}(T_{in}) - p)/p_{sat}(T_{in})$. The 296 HRM model and the relaxation time correlation of [119] has been widely 297 adopted in the computational fluid dynamics modelling of flash-boiling 298 atomization, e.g. [3, 104–107], while less in the nuclear safety analysis. 299 Similar relaxation times may be derived for other thermodynamic param-300 eters, and they may differ. Bilicki et al. [123] presented a method for the 301 evaluation of the relaxation time of interphase heat exchange. Moham-302 madein [124] derived a formula for the thermal relaxation time by solving 303 energy and relaxation equations analytically, in terms of two-phase mix-304 ture between two finite temperatures boundaries. 305

• Delayed Equilibrium Model (DEM): In comparison to others, the delayed equilirium model (DEM) is not widely used. For the sake of completeness, it is introduced briefly here. The basic idea of the DEM for describing the flashing flow is that the mixture is composed of three phases, i.e. saturated liquid, saturated vapor and metastable liquid [108]. The third phase is in thermal non-equilibrium with the saturated ones, while the whole mixture is at pressure and mechanical equilibrium. The expansion

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of the metastable liquid is an isentropic process. In addition to the mixture 313 system of equations, an extra mass balance equation for the metastable 314 liquid phase is solved. De Lorenzo et al. [109] benchmarked the DEM 315 model and other three well-known two-phase critical flow models, namely, 316 the HEM model, the Moody NHEM model [27] and the Henry-Fauske 317 HNEM model [28], against more than 450 experimental data. The results 318 showed that none of the classical models can be considered as a general 319 method for the evaluation of the two-phase critical flow. Although positive 320 results in evaluating the critical mass flow rate of long tubes, HEM fails in 321 predicting the critical pressure. Moody's model is unsuitable under two-322 phase stagnation conditions. The Henry-Fauske model provides rather 323 good results for nozzles and orifices, but overestimates the critical mass 324 flow in long tubes. On the other hand, DEM exhibits reliable results for 325 the configurations ranging from long and short tubes to narrow slits in 326 terms of both critical pressure and critical mass flux. 327

• Physically-based models: As aforementioned, thermal non-equilibrium 328 processes in a flashing flow concern nucleation and interphase heat trans-329 fer. Some works consider both of them, while others only the latter by 330 prescribing a constant bubble number density. Despite numerous attempts 331 have been made, limited understanding of the physical phenomena pre-332 vent from defining the non-equilibrium effects precisely. So, it can happen 333 that the results obtained from a physically-based model are worse than 334 those from a simpler one [21, 125]. The non-equilibrium models can be 335 incorporated with homogeneous, drift-flux or two-fluid models in one or 336 more spatial dimensions. Within the context of a one-dimensional homo-337 geneous model, Wolfert et al. [43] simulated three blowndown experiments 338 by focusing on the interphase heat transfer, which determines the vapor 339 generation rate. The overall transfer coefficient was calculated by combin-340 ing the heat diffusion model of Plesset and Zwick [126] and the convection 341 model of Ruckenstein [127] cumulatively. Furthermore, they took into 342

account the turbulence enhancement by introducing an eddy conductiv-343 ity. The bubble number density was treated as a constant, needed to 344 be adjusted from case to case. For the modelling of flashing flow in a 345 converging-diverging nozzle, Wu et al. [31] attempted to find out the 346 flashing inception location by using the semi-empirical onset correlation 347 of Alamgir and Lienhard [4]. Downstream from the onset location, a con-348 stant number of bubbles was assumed, and the bubbles initially have the 349 critical size corresponding to the onset pressure. The vapor generation 350 rate was assumed to be limited by heat conduction and calculated from 351 the correlation proposed by Plesset and Zwick [126]. The lack of under-352 standing of the heterogeneous nucleation process remains one difficulty 353 in the modelling of flashing flows. Rohatgi and Reshotko [110] simulated 354 flashing liquid nitrogen flow in a venturi using a one-dimensional HNEM 355 model. They accounted for heterogeneous nucleation by making analogy 356 to the classical homogeneous nucleation theory with the assumption that 357 nucleation in the bulk is dominant. Two adjustable parameters are con-358 tained in their model, one being the value of activated nucleation site 359 density and the other being the heterogeneity factor. Blinkov and his 360 co-workers developed a quasi-one-dimensional HNEM model to calculate 361 the behavior of nucleation and flashing in nozzles [111]. Besides the mix-362 ture conservation equations, one continuity equation for the vapor phase 363 and one transport equation for the bubble number density were solved. 364 Both bulk and wall nucleation phenomena were considered. Heteroge-365 neous nucleation in the bulk was modelled by assuming a size distribution 366 of pre-existing nucleation sites, and the activated nucleation site density 367 is correlated with the Gibbs number. A cavity model was proposed for de-368 termination of the nucleation site density, bubble departure diameter and 369 frequency at the wall. Deligiannis and Cleaver[112] considered the effect 370 of homogeneous and heterogeneous nucleation in the frame of a two-fluid 371 model with zero slip between the phases. 372

373 2.4. NHNEM models

Besides above homogeneous models, the non-equilibrium effects regarding nucleation and interphase heat transfer are often considered in the context of non-homogeneous models, where the velocity difference between the gas and liquid phases is taken into account by using the drift-flux or two-fluid model. [30, 32, 102, 113]

• Drift-flux model: Kroeger [102] applied a non-equilibrium drift flux model 379 to two-phase blowdown experiments. The vapor generation rate was cal-380 culated from a relaxation type model, and the vapor drift was considered 381 by the correlations proposed by Zuber and Findlay [128]. Another non-382 equilibrium drift flux model was presented in Elias and Chambé [113]. 383 They assumed that the evaporation rate is governed by interphase heat 384 transfer. The evaporation rate is determined by a conduction bubble 385 growth model[129], while the convection effect is negligible. A similar 386 non-equilibrium model was developed by Saha and his co-workers [30], 387 and the major difference lies in modelling of interphase heat transfer. 388 Saha et al. stated that the Plesset-Zwick or Forster-Zuber type of heat 389 transfer coefficient may be applicable for short time after nucleation. As 390 the bubbles "age", convection starts to dominate the heat transfer because 391 of the relative velocity between the bubbles and liquid. They used a sim-392 ple expression which provides the root mean square of the conduction and 393 convection heat transfer coefficients [130]. Riznic et al. [32] improved the 394 drift-flux model by considering bubble generation and transportation in-395 stead of assuming a constant bubble number density. The bubble number 396 transport equation was solved with a distributed source from wall nucle-397 ation. In addition, they took into account the variable pressure effects in 398 their conduction bubble growth model according to the results of Jones 399 and Zuber [131]. They found that in a variable pressure field, which cause 400 the saturation temperature to vary as t^n (t being time), the bubble radius 401 will grow as $t^{n+1/2}$. It is significantly faster than $t^{1/2}$ usually expected for 402

the initial superheat.

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• Two-fluid model: Saha et al. [30] recognized that a two-fluid model is 404 superior to the drift-flux model for calculating relative velocity. One-405 dimensional two-fluid equations were used by Ardron [132] for the cal-406 culation of critical flow in a pipe. The nucleation and diffusion-limited growth of vapor bubbles in superheated liquid were considered in the de-408 termination of vapor generation rate. The nucleation rate was computed 409 based on the classical nucleation theory by introducing a heterogeneity 410 factor. A similar model was presented in [110], where the density of nucle-411 ation sites and the heterogeneity factor are two adjustable parameters. By 412 neglecting the sphericity of the bubble and assuming linear time variation 413 of the liquid superheating degree, the diffusive heat flux from the thermal 414 boundary to the bubble wall was approximated as 415

$$q_i(t,t') = \frac{\lambda_l}{\sqrt{\pi a_l(t-t')}} \left[2T_{sup}(t) - T_{sup}(t')\right]$$
(1)

where t' is the time point at which the bubble is created, λ_l abd a_l are 416 liquid thermal conductivity and diffusivity. Rivard and Travis [133] de-417 scribed the vapor production and bubble growth by the well-known heat 418 diffusion controlled rate presented in [126], but considered the enhance-419 ment in thermal diffusivity due to the effect of relative motion and liquid 420 turbulence, i.e. $a_{eff} = a_l + Ar_B U_{rel}$, where $a_{eff}, a_l, r_B, U_{rel}$ is effective 421 diffusivity, molecular diffusivity, bubble radius and relative velocity, re-422 spectively, and A is an empirical constant. In addition, a constant bubble 423 number density $N = 10^9 m^{-3}$ was specified and nucleation was neglected. 424 Richter^[29] applied the two-fluid model to calculation of critical flow rates 425 for steam-water mixtures from nozzles. He postulated that convection 426 is the dominant mode of interphase heat transfer during flashing, and 427 adopted the empirical correlation proposed by Ranz and Marshall [134] for 428 estimation of heat transfer coefficient in the bubbly flow regime. Different 429 flow regimes were considered in the model, like bubbly, churn-turbulent 430

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and annular. The transition from one regime to another was assumed to 431 occur at certain void fractions. A similar two-fluid model was presented in 432 [125], while different correlations were used for the constitutive equations, 433 i.e. drag coefficient and heat transfer coefficient. Schwellnus [135] included 434 a seventh equation for bubble diameter up to the point from bubbly to 435 churn-turbulent flow. The bubble number density was updated basing on 436 the bubble diameter and void fraction. For the purpose of analyzing crit-437 ical flows in pipes of nondiverging cross-sectional area, Dagan et al. [136] 438 derived an empirical correlation for the number density of bubbles as a 439 function of pipe's length to diameter ratio. Furthermore, they extended 440 the conduction bubble growth model proposed by Olek et al. [137] to in-441 clude the convection effects. Tiselj and Petelin [33] simulated the critical 442 flashing flow in a converging-diverging nozzle with the two-fluid model in 443 RELAP5. The simulation results were compared with the experiments 444 performed in the BNL laboratory [26]. They pointed out that the major 445 source of discrepancies is the neglect of the flashing delay. Recently, Koz-446 menkov et al. [81] and Atajafari et al. [114] validated the RELAP5 code 447 for FII observed at the CIRCUS [72] and SIRIUS-N [73] test facilities, 448 respectively. Wein [115] developed a two-fluid model for flashing flows of 449 initially subcooled and saturated fluids through pipes and nozzles. It con-450 sists of six conservation equations of mass and momentum, liquid thermal 451 energy and bubble number transport. Constitutive equations describing 452 interphase mass, momentum and heat transfer account for different flow 453 regimes. Nucleation on the wall and in the bulk flow was considered. 454 The results proved that the importance of fluid dynamic non-equilibrium 455 increases with vapor volume fraction. 456

457 3. Computational fluid dynamics modelling

⁴⁵⁸ Multi-dimensional CFD-based simulations are becoming a useful tool for ⁴⁵⁹ studying transients, instabilities and phase transitions in two-phase flow sys-



Figure 1: Vertical circular convergent-divergent nozzle in BNL experiments [26]

tems [118]. Since the beginning of the 2000s there arise a number of CFD 460 works on flashing flow related to the nuclear reactor safety problems. Insights 461 to smaller scale flow processes which were not seen by system codes may be ac-462 quired by using the CFD tool. It brings a better understanding of local physical 463 phenomena, more confidence in the results and then better definition of safety 464 margins. However, the same problem as in one-dimensional codes encountered 465 here is that, constitutive models are not as mature as in single phase flows, and 466 a general consensus regarding model selection is not available. A lot of work 467 has still to be done on the physical modelling and numerical algorithm [138]. 468

469 3.1. Flashing nozzle flow

CFD simulation of flashing flows in nuclear applications are mostly concen-470 trated on the steady-state nozzle flow or critical (chocked) flow. Considering 471 that the BNL experiments [26] have been frequently simulated, geometrical de-472 tails about the nozzle and some test runs are presented in Figure 1 and Table 473 2, respectively. In most cases the mass flow rates obtained using different mod-474 els conform well with the data, although adjustment of some parameters such 475 as the accommodation coefficient [41] and the bubble number density [40] was 476 often necessary. Details about the numerical methods and models adopted in 477 each work are discussed below. 478

⁴⁷⁹ Maksic and Mewes [35] examined the flashing flow in the BNL nozzle [26]
⁴⁸⁰ by performing simulations with the commercial CFD-code ANSYS CFX version
⁴⁸¹ 4.2. The simplified two-phase model consists of continuity and momentum equa-

$\operatorname{Run}\#$	p_{in} [kPa]	p_{out} [kPa]	T_{in} [K]	$\dot{m}_{exp} \; [\rm kg/s]$	$\dot{m}_{cal} \; [\rm kg/s]$
122	171.0	109.2	373.35	6.12	6.25 [36]
128	248.0	101.0	373.15	9.13	8.78 [36]
100	240.0	202.0	204.25	0.0	9.2 [40]
133	349.0	203.0	394.35	9.0	$8.80 \ [36]$
137	464.0	208.9	394.75	11.95	12.1 [40]
1 4 5	202.0	200 5	204.25		7.7 [40]
145	306.0	208.7	394.35	7.52	7.37 [37]
	224.0	20.0.0	204.25		7.50 [36]
148	304.0	206.0	394.35	7.52	7.33 [37]
					8.4 [40]
268	575.2	443	422.05	8.74	9.20 [41]
					9.10 [139]
273	573.5	442.1	421.85	8.72	8.3 [40], 8.85 [35]
					$8.51 \ [37], \ 9.30 \ [41]$
278	688.6	434.1	421.95	11.67	10.9 [40], 12.30 [41]
284	530.1	456.0	422.35	7.30	7.0 [40], 7.70 [41]
288	530.8	456.3	422.25	7.26	7.12 [37]
291	504.7	470	422.05	6.44	6.1 [40]
296	764.9	432.6	421.95	13.13	12.4 [40], 13.90 [41]
304	577.7	441	422.15	8.76	9.1 [40], 9.10 [41]
					8.4 [40], 8.75 [36]
309	555.9	402.5	422.25	8.80	7.56 [37], 8.80 [41]
					8.72 [139]
344	539.9	190.0	394.15	13.47	12.7 [40]
348	226.9	199.4	394.35	4.57	4.30 [37]
358	370.2	101.2	373.15	12.13	11.5 [40]
362	443.3	101.2	372.85	13.68	12.9 [40]

Table 2: Operational conditions and test runs in BNL experiments [26]

tions for the mixture of liquid and vapor, a separate continuity equation for the 482 vapor and an energy equation for the liquid. The vapor phase was assumed to 483 be saturated, and its temperature was calculated from the local pressure. The 484 four-equation HNEM model was supplemented with a transport equation for the 485 bubble number density. Both bubble sizes and numbers were allowed to change 486 in this way. The generation of bubbles from wall nucleation was considered, and 487 the nucleation rate was calculated according to the Jones model [111, 131]. The 488 surface source was transformed to a volumetric source by multiplying it with 489 the ratio of the pipe perimeter to the cross-sectional area of the pipe $\frac{\xi}{A}$, i.e. 490

$$J_w = N_w f_w \frac{\xi}{A} \tag{2}$$

where N_w, f_w denotes the nucleation site density and nucleation frequency at 491 the wall, respectively. The transformation in Eq. (2) may lead to inconsistency, 492 since N_w has a value of zero everywhere except in the cells adjacent to the 493 wall. For the calculation of interfacial area density, the authors considered two 494 regimes, bubbly regime ($\alpha < 0.3$) and slug regime (($\alpha > 0.3$)). In the slug 495 flow regime, the interfacial area density was assumed to be the sum of that of 496 spherical bubbles and cylindrical slugs, but the volume fraction of each type 497 of the bubbles was not provided. The interfacial heat transfer was assumed 498 to be dominated by heat conduction, and the Nusselt number is a function of 499 the Jakob number. The empirical correlation presented by Labuntzov [140] was 500 adopted. 501

$$Nu = 2 + \frac{12}{\pi} Ja + \left(\frac{6Ja}{\pi}\right)^{1/3}$$
(3)

⁵⁰² The Jakob number is defined by

$$Ja = \frac{c_{pl}\rho_l \Delta T_{sup}}{\rho_v H_{lv}} \tag{4}$$

where c_{pl} is the isobaric heat capacity of liquid. For the test run 273 with inlet pressure of 573.5 kPa, temperature of 421.85 K, see Table 2, a good agreement on the mass flow rate was achieved. However, the simulation showed a fluctuating pressure profile in the diverging part of the nozzle, and underpredicted the void fraction in the diverging part of the nozzle.

Marsh and O'Mahony [37] simulated the same nozzle flow using a full two-508 fluid model in the commercial CFD code ANSYS FLUENT, with separate mass, 509 momentum and enthalpy balance equations for liquid and vapour. Inter-phase 510 mass and momentum as well as energy transfer resulting from both nucleation 511 and phase change were taken into account. However, the effect of non-drag forces 512 on the momentum exchange and heat transfer between the vapor and vapor-513 liquid interfaces were neglected. Like in the previous work vapor generation 514 is determined from interphase heat transfer, but information about the heat 515 transfer coefficient is not provided. The generation of bubbles from nucleation 516 was taken into account by solving a bubble transport equation. The nucleation 517 rate was computed by a modified version of the Blander and Katz model [141]. 518

$$J_w = N^{2/3} S\left(\frac{2\sigma N_A}{\pi m_w B}\right)^{1/2} exp\left(-\frac{\phi}{(T_{sat} - T_l)^n}\right)$$
(5)

where N is the number of liquid molecules per unit volume, and the power 2/3519 is to transform it to a surface density, m_w is the molecular weight and $S = (1 - 1)^{-1}$ 520 $(m_w)/2, N_A$ is the Avogadro number, σ is the surface tension coefficient, and B 521 is a constant having a value of 2/3 in case of flashing. The exponential term was 522 written in terms of superheat instead of pressure undershoot as in the original 523 model for the sake of numerical stability. In addition to the heterogeneous 524 factor ϕ an adjustable constant n was introduced. Details on how to convert 525 the surface flux J_w to the volumetric source required by the bubble transport 526 equation are not provided. The calculated and measured mass flow rate was 527 compared for six BNL runs carried out by Abuaf et al. [26], see Table 2. Good 528 agreement was achieved for all cases except Run 309, which has a high inlet 529 pressure and a relatively low outlet pressure, in other words high vaporization 530 rate. Furthermore, in contrast to that a bubble layer in the vicinity of the wall 531 as reported in [35], the distribution of vapor in the diverging part of the nozzle 532 is almost uniform. The difference mainly results from the nucleation models 533

that are applied. The model of Blander and Katz [141] was derived from the classical nucleation theory for bulk nucleation and activated not only on the walls but all over the domain depending on local liquid superheat. It differs in nature from the Jones wall cavity model [111] used in the previous work.

The disagreement on nucleation modelling motivated Janet et al. [39] to 538 evaluate the existing models. They analyzed the heterogeneous nucleation ef-539 fects in the BNL nozzle using the two-fluid model in ANSYS CFX 15.0. As in 540 the work of Maksic and Mewes [35], the vapor and vapor-liquid interface were 541 assumed to remain saturated by applying the zero resistance model, but sepa-542 rate velocity fields were solved for the liquid and vapor phases. To estimate the 543 heat transfer between the superheated liquid and the interface, the correlation 544 of Aleksandrov [142] was used. It combines the heat diffusion and convection in 545 the following way: 546

$$Nu = \left(\frac{12}{\pi^2} J a_T^2 + \frac{1}{3\pi} P e\right)^{1/2} \tag{6}$$

where Pe is the Péclet number. Like in [35, 37] a transport equation was solved 547 additionally for the bubble number density. The nucleation source was imple-548 mented as a boundary flux into the near-wall mesh cells. Three wall nucleation 549 models, i.e. the Jones model [111, 131], the RPI model [143] and Riznic model 550 [32], were investigated. The performance of the models was found to differ qual-551 itatively and quantitatively in predicting of the bubble departure frequency and 552 diameter along the nozzle. The Jones model predicted the best agreement on 553 the mass flow rate. Considering only wall nucleation leads to the same profile 554 as observed in [35], i.e. a bubble layer appearing in the vicinity of the wall, 555 whose thickness increases along the nozzle axis, while the void fraction in the 556 central part of the nozzle is nearly zero. On the other hand, the measured pro-557 files show non-zero values in the central region along with high peaks near the 558 wall. Based on this observation, Janet et al. [39] suggested that both wall and 559 bulk nucleation play a role in flashing nozzle flows although wall nucleation is 560 dominant in most cases. The effect of bulk nucleation was considered by using 561

the model proposed by Rohatgi and Reshotko [110]. The bulk nucleation rate is given by

$$J_b = N_b \left(\frac{2\sigma}{\pi m_w}\right)^{1/2} exp\left(-\frac{16\pi\sigma^3\phi}{3\kappa T_l(p_{sat} - p_l)^2}\right)$$
(7)

where N_b is the number density of liquid molecules, p_{sat} is the vapor pressure at the liquid temperature and κ is the Boltzmann constant. Considering both wall and bulk nucleation improves the agreement between the measured and simulated radial profiles considerably.

The nucleation region in above BNL nozzle test runs has been shown suffi-568 ciently narrow (a few centimeters) both experimentally [31] and numerically [39]. 569 The bubble number density is nearly constant after the nucleation region. Based 570 on these observations Liao and Lucas [40] revisited these cases with prescription 571 of the bubble number density. The initial tiny bubbles can be deemed as pre-572 existing germs, which start to grow as long as the surrounding liquid becomes 573 saturated. This is a major difference from the numerical model applied in the 574 previous work of [39], where the nucleation delay was considered. Fourteen cases 575 with different inlet/outlet pressures and temperatures were benchmarked. The 576 error between predicted mass flow rates and experimental data for all cases was 577 below 7%, see Table 2. At the same time, satisfying agreement regarding axial 578 profiles of void fraction and pressure was observed, which are greatly improved 579 in comparison with the one-dimensional results published in [31]. However, 580 the lateral distribution of bubbles reveals large discrepancy, although non-drag 581 forces including lift, added mass, turbulence dispersion and wall lubrication are 582 considered [144]. Both simulation and experiment gives a wall-peak profile, 583 but the predicted void fraction in the central region is much too high. It evi-584 denced that dynamic processes such as bubble nucleation, growth, coalescence 585 and breakup were not reproduced by the numerical model appropriately, apart 586 from the uncertainties in the force models. To capture the lateral bubble migra-587 tion, a poly-disperse approach tracing the local bubble size change is necessary. 588 Mimouni et al. [145] simulated one critical flow case of the Super Moby 589

Dick experiment [146] with the NEPTUNE_CFD solver. It has the boundary 590 conditions of 39.96 bars at the inlet and 23.176 bars at the outlet, and the initial 591 water subcooling is of about 10°C. Mass, momentum and energy balance equa-592 tions are solved for both liquid and vapor. The interfacial transfer of momentum 593 consisted of three forces, i.e. drag, virtual mass and the secondary momentum 594 source associated with the interfacial mass transfer. Nucleation occurring at the 595 wall and pre-existing germs are considered. The former is modelled by using 596 the Jones nucleation model [111], while the latter by presuming an initial void 597 fraction. In addition, the original correlation for the nucleation site density was 598 modified for sake of generality. The change of bubble size and number density 599 was not solved, and instead, a constant value was prescribed for the bubble size. 600 The heat transfer coefficient on the vapor side was set to a large value to ensure 601 the vapor temperature remaining very close to the saturation temperature, and 602 on the liquid side was calculated using the Ranz-Marshall correlation [134]. 603

$$Nu = 2.0 + 0.6Re_n^{1/2}Pr_l^{1/3} \tag{8}$$

While the majority of investigations indicated that the wall nucleation is 604 predominant in flashing flows, Mimouni et al. [145] found the vapor genera-605 tion at the wall negligible in comparison to that from pre-existing nuclei. The 606 inconsistency is caused by the fact that the pre-existing nuclei are activated 607 earlier (at saturation conditions) and suppress the activation of nuclei on the 608 walls. It can be expected that the void fraction in the central region would be 609 over-predicted as shown in [40]. The effect of initial void fraction as well bubble 610 size was discussed. Taking into account the poly-dispersity was identified as one 611 important issue requiring further efforts. 612

In all above investigations phase change was deemed driven by thermal difference, and the bubble growth and vapor generation rate was determined by modelling the interfacial heat transfer process. Similar for nucleation models, a broad consensus on choosing interphase heat transfer models does not exist. In some works conduction was assumed to be a predominant heat transfer mechanism, while in others convection. An evaluation of the heat transfer coefficient models for flashing flows was conducted by Liao and Lucas [130]. They attempted to generalize the model by taking into account convection and turbulence effects along with the conduction, and validated it for condensing and evaporating flows [130, 147].

On the other hand, a few CFD works on the flashing nozzle flow assumed 623 that phase change is controlled by pressure difference, and applied a conven-624 tional cavitation model derived from the R-P (Rayleigh-Plesset) equation. For 625 example, Palau-Salvador et al. [36] simulated the BNL nozzle flow [26] using 626 the cavitation model of Singhal et al. [148] available in the CFD code ANSYS 627 FLUENT 6.1. The model assumes that the flow is isothermal. Pre-existing 628 germs start to grow as local pressure drops below the saturation pressure, and 629 collapse in the reverse case. Mass and momentum balance equations are solved 630 for the mixture of liquid and vapor. Like in [35], a transport equation was 631 solved for the vapor fraction besides the mixture conservation equation, and the 632 source terms representing bubble growth and collapse are described by the R-P 633 equation. 634

$$\dot{\Gamma} = \begin{cases} C_{vap} \frac{\max(1.0, \sqrt{k})(1 - f_v - f_g)}{\sigma} \rho_l \rho_v \sqrt{\frac{2(p_v - p)}{3\rho_l}} & \text{if } p \le p_v , \\ -C_{cond} \frac{\max(1.0, \sqrt{k}) f_v}{\sigma} \rho_l \rho_l \sqrt{\frac{2(p - p_v)}{3\rho_l}} & \text{if } p > p_v. \end{cases}$$
(9)

⁶³⁵ Wherein f_v , f_g are mass fraction of vapor and non-condensable gases, k is tur-⁶³⁶ bulent kinetic energy, C_{vap} , C_{cond} are two empirical coefficients having a unit ⁶³⁷ of m/s. The local turbulence effect on the saturation pressure is considered by ⁶³⁸ considering an additional turbulent fluctuation:

$$p_v = p_{sat} + 0.195\rho k \tag{10}$$

Five BNL test runs from [26] were validated, see Table 2. Good agreement between the measured and calculated mass flow rates was achieved with a difference less than 4%. Satisfying prediction of axial pressure and vapor fraction

was shown for one case, where the thermal non-equilibrium effect at the onset 642 of flashing is not that significant. As expected from the homogeneous mixture 643 model, the contour plot of void fraction exhibits a uniform distribution of vapor 644 in the lateral direction of the nozzle, which is inconsistent with the experimen-645 tal observation as discussed above. Another cavitation model in the ANSYS 646 FLUENT code, i.e. the Schnerr and Sauer model [149], was utilized by Ishigaki 647 et al. [150] for analyzing the two-phase critical flow in nozzles and breaks. The 648 Super Moby Dick experiment [146] and the SGTR experiment at Large Scale 649 Test Facility (LSTF) of Japan Atomic Energy Agency [151] were simulated. 650 The authors concluded that the CFD code ANSYS FLUENT has the possibil-651 ity for simulation of two-phase critical flows related nuclear safety analysis. The 652 physical properties were shown to have a significant influence on the flow rate 653 predictions, and an more accurate estimation is necessary. The authors treated 654 the vapor as an ideal gas, and calculated the density of liquid according to the 655 Tait equation of state. In contrast, the simulations performed in ANSYS CFX 656 mostly use the IAPWS-IF97 formulation of the thermodynamic properties of 657 water and steam. 658

On the other hand, Liu et al. [38] pointed out that above isothermal cavita-659 tion models cannot be used for flashing flows directly, because the dependency 660 of vapor generation rate on temperature variations is usually non-negligible 661 under the high temperature and pressure conditions. They constructed a so-662 called thermodynamic cavitation model based on the homogeneous multiphase 663 model with common flow fields shared by all fluids including temperature and 664 turbulence. In order to take into account the thermal effects in flashing, the 665 dependency of fluid physical properties on the temperature was introduced, e.g. 666 the saturation vapor pressure, surface tension as well liquid and vapor densities, 667 using empirical formulas. The mass transfer source terms related to bubble 668 growth and collapse were derived based on the H-K (Hertz-Knudsen) formula, 669 which gives the evaporation-condensation flux based on the kinetic theory on a 670

671 flat interface.

$$\dot{\Gamma} = \begin{cases} F_{vap} \frac{6(1 - f_v - f_g)}{d_B} \frac{2\sigma}{2 - \sigma} \sqrt{\frac{M}{2\pi RT}} (p_v - p) & \text{if } p \le p_v , \\ -F_{cond} \frac{6f_v}{d_B} \frac{2\sigma}{2 - \sigma} \sqrt{\frac{M}{2\pi RT}} (p - p_v) & \text{if } p > p_v. \end{cases}$$
(11)

where M is the molar mass of liquid, R is the gas constant, T is the mixture 672 temperature, and F_{vap} , F_{cond} are two adjustable constants. The contribution of 673 turbulent fluctuation to the pressure variation was considered according to Eq. 674 (10). The authors simulated one BNL nozzle test run with the modified cavita-675 tion model, and compared the simulation results with those presented in [36]. A 676 minimal improvement of the axial void fraction profile was indicated. Further-677 more, it showed surprisingly that the vapor volume fraction at the temperature 678 of $100^{\circ}C$ is higher than $150^{\circ}C$. It implies that the way how the thermal effect 679 was considered is inappropriate. 680

Le et al. [41] investigated the BNL nozzle flow experiments by implementing a similar model as [38] in the commercial code ANSYS FLUENT 16.2. The source term for the mass flux at the interface is derived according to the H-K formula,

$$\dot{\Gamma} = A_i \beta \sqrt{\frac{M}{2\pi R T_{sat}}} \left(0.195\rho k + p_{sat} - p * \right)$$
(12)

where β is the so-called "accommodation" coefficient taking into account the 685 thermal non-equilibrium effects partially. The interfacial area density A_i is 686 modelled by assuming a constant bubble number density as in [40]. The source 687 term was inserted by means of a user-defined function. The coefficient β as 688 well the pressure difference $dp = p_{sat} - p*$ was treated as adjustable constants 689 in the simulation. The model was validated against experimental data [26] 690 and numerical results of previous work [39, 40]. The discrepancies between 691 the measured and simulated radial vapor profiles were attributed to the two-692 phase mixture approach and the slip model, which makes use of an algebraic 693 slip relation for the relative velocity. A two-fluid model along with a complete 694

⁶⁹⁵ modelling of the thermal effects was recommended.

In the frame of a homogeneous mixture model Jin et al. [139] included source and sink terms of interfacial mass transfer induced by both pressure and thermal difference ($\dot{\Gamma} = \dot{\Gamma}_p + \dot{\Gamma}_T$). The pressure phase change model has a similar form as Eq. (11) and Eq. (12), i.e.

$$\dot{\Gamma}_{p} = \begin{cases} F_{vap} \frac{\rho_{v} f_{l}}{t_{ch}} min\left(1, \frac{p_{v} - p}{k_{p} p_{v}}\right) & \text{if } p \leq p_{v} ,\\ -F_{cond} \frac{\rho_{v} f_{v}}{t_{ch}} min\left(1, \frac{p - p_{v}}{k_{p} p_{v}}\right) & \text{if } p > p_{v}. \end{cases}$$

$$(13)$$

where t_{ch} is the characteristic flow time, k_p is a scaling constant that determines the pressure level at which the vaporization model comes into effect. The thermal mass transfer rate was calculated according to the thermal phase change model presented by Lee [152].

$$\dot{\Gamma}_{T} = \begin{cases} F_{vap} \frac{\rho_{l} f_{l}}{t_{ch}} \frac{(T - T_{v})}{T_{v}} & \text{if } T > T_{v} ,\\ -F_{cond} \frac{\rho_{v} f_{v}}{t_{ch}} \frac{(T_{v} - T)}{T_{v}} & \text{if } T \le T_{v} . \end{cases}$$

$$(14)$$

The model was implemented in a in-house CFD code, whose capability of simulating flashing flows was assessed by studying the BNL nozzle flow. Two test runs (309 and 268) were simulated, and good agreement in terms of axial profiles of pressure and void fraction was achieved.

Schmidt et al. [3] extended the classical one-dimensional closures for the HRM model proposed by Downar-Zapolski et al. [119], to multiple dimensions, and implemented them in the open source CFD code OpenFOAM. The solver was firstly validated for a case taken from Tikhonenko et al. [153], who explored flashing critical flow in various pipes with a sharp inlet. These experiments include pressure measurements along the length of the pipe. High-pressure and low-pressure correlations for the relaxation time Θ were tested.

$$\Theta = \begin{cases} 6.51 \times 10^{-4} \alpha^{-0.257} \psi^{-2.24} & \text{if } p \le 10 \text{bar} ,\\ 3.84 \times 10^{-7} \alpha^{-0.54} \phi^{-1.76} & \text{if } p > 10 \text{bar}. \end{cases}$$
(15)

715 where the definitions for ψ and ϕ are

$$\psi = \left| \frac{p_{sat} - p}{p_{sat}} \right| \tag{16}$$

$$\phi = \left| \frac{p_{sat} - p}{p_c - p_{sat}} \right| \tag{17}$$

where p_c denotes the critical pressure. Both correlations were found to under-716 predict the flashing rate, and the low-pressure correlation is especially far off. 717 The second test case was taken from the experiments conducted by Fauske [154], 718 in a relatively short and small tube. In this case, surprising good agreement on 719 the mass flow rate was achieved by the low-pressure correlation, while the high-720 pressure correlation under-predicted by a factor of two. The authors concluded 721 that future development should focus on developing a general correlation for the 722 relaxation time, and considering non-homogeneous, turbulence and nucleation 723 effects. 724

Similar attempts extending a one-dimensional model to multi-dimensions 725 were made by Duponcheel et al. [155]. They implemented and the DEM model 726 in the NEPTUNE_CFD multi-field solver, and tested it for flashing chocked 727 flows. The validation cases were taken from the Super Moby Dick experiments 728 [146]. Two inlet conditions were simulated: $T_{in} = 240.5 \ ^{o}C$ and $T_{in} = 249.4 \ ^{o}C$. 729 The homogeneous condition, i.e. identical velocities for all the phases, is ob-730 tained by adding very large drag forces. The saturated liquid and vapor were 731 constrained to remain saturated by adding strong interfacial heat transfer terms. 732 The metastable liquid phase was considered "frozen", and no interfacial heat 733 transfer with the saturated phases. The mass transfer from the metastable liq-734 uid to the saturated liquid was determined by using an empirical correlation. 735 The implemented model was able to give good agreement for the case closer to 736 saturation, but under-predicted the mass flow rate by 13.5% in case of larger 737 inlet subcooling. Yet, in both cases the multi-dimensional results are worser 738 than the one-dimensional ones using the original DEM. 739

740

As shown above various phase-change models have been adopted for the pre-



Figure 2: Comparison between simulation results from literature for BNL test case 309 [4]. (a) Axial void fraction profile (b) Axial pressure profile

diction of flashing flows, e.g. thermal phase-change model based on temperature 74 difference (TPCM) and pressure phase-change model based on pressure differ-742 ence (PPCM). The PPCM models can be divided further into two categories, 743 i.e. based on the kinetic theory of gases (H-K equation) and based on bub-744 ble dynamics (R-P equation). A comparative evaluation of these models was 745 performed by Karathanassis et al. [156] together with the two-phase mixture 746 model in ANSYS FLUENT 14.5. The results showed that the phase-change 747 model based on the kinetic theory of gases produced accurate predictions for 748 all the cases investigated ("Super Moby Dick" nozzle [23], "Reitz" nozzle [157], 749 "Edwards" pipe blowdown [42]), while the validity of HRM and model based 750 on the R-P equation was found situational. Similar results were presented in 751 [158], which showed that the PPCM model based on the R-P equation failed in 752 reproducing the pressure undershoot phenomenon and simulating the thermal-753 controlled phase change. For the BNL test case run 309 as an example, Figure 2 754 compares the prediction of axial void fraction and pressure profile using differ-755 ent models with the experimental data. The void fraction provided by Le et al. 756 [41] conforms well with the measurement, while the pressure profile of Liao and 757 Lucas [40] gives the best agreement. In comparison to axial profiles, prediction 758 of the lateral distribution of void fraction is even more challenging. 759

760 3.2. Pipe blowdown

Jo et al. [159, 160] investigated water flashing flow from a PWR steam 761 generator (SG) by a feed water line break (FWLB) accident using the com-762 mercial CFD code ANSYS CFX. The simplified SG model and broken position 763 is sketched in Figure 3(a). The space occupied by the tube bundle in the SG 764 secondary side was simulated with the porous medium model. The discharge 765 flow accompanying with thermal phase change was calculated by employing the 766 NHNEM two-fluid model, governing equations were solved for the liquid and 767 vapor phases separately. The gas phase consisted of discrete spherical bubbles 768 with a uniform size. The $k - \omega$ SST model was used to estimate the turbulent 769 viscosity. The phase change was driven by temperature difference and inter-770 phase heat transfer. Transient pressure, velocity, void fraction response of the 77 SG secondary side and the broken pipe side was analyzed. Vapor was built 772 firstly at the exit of the broken pipe, and developed along the pipe wall with 773 a liquid core towards SG. The FWLB accident resulted in steep escalation of 774 the SG secondary flow velocities, especially near the broken pipe. Figure 3(b) 775 plots the mixture velocity responses at four monitoring points for the first 0.3 776 s, where the distance to the broken position decreases from point 1 to point 4. 777 At the exit of the broken nozzle (point 4), the velocity is over 100 m/s, which 778 may cause mechanical damage on some tubes. The authors investigated the 779 effect of initial state of the fluid upstream the broken pipe end, i.e. subcooled 780 water, saturated steam or saturated water-steam mixture. It was found that 781 the subcooled water non-flashing flow model gives the maximum discharge flow 782 rate, the saturated water flashing flow model the minimum, while the sub-cooled 783 water flashing flow model ranges between. In addition, the simulation results 784 were shown to have a sensitive dependence on the initial interfacial area density 785 related to the choice of gas volume fraction and bubble mean diameter. 786

Karathanassis et al. [156] presented CFD simulations of flashing flow from the Edwards pipe blowdown [42] in addition to two discharge nozzles. A sketch of the pipe as well as the measurement points (P1 \sim P7) is depicted in Figure 4. As aforementioned their numerical studies were based on the two-phase



Figure 3: CFD simulation of FWLB induced discharge flow from SG [160]. (a) Simplified SG model (b) Transient velocity response at different monitoring points: Point 1 (SG center at the broken pipe level), Point 2 (first upstream point of the broken pipe in SG), Point 3 (second upstream point of the broken pipe in SG), Point 4 (center of the cross-section at the mid point of the broken pipe)



Figure 4: Sketch of the Edwards blowdown experiments [42]

mixture model assuming zero slip velocity. They evaluated the capability of 791 various mass-transfer rate models. The interfacial area density A_i was calculated 792 assuming a nucleation site density of $10^{13} m^{-3}$ and a bubble radius of $10^{-6} m$. 793 In other words, A_i remains constant during the phase change process, which 794 deviates obviously from the physical picture. For the blowdown case, three 795 formulations of the PPCM model based on the H-K equation, i.e. HK1, HK2, 796 HK3, were compared with the HRM model. The HK2 model computes the 797 interfacial mass flux in a way similar to Eq. 12, while in HK1 it is simplified as 798

$$\dot{\Gamma} = A_i C_{evap} \alpha_l \rho_l \left(0.195 \rho k + p_{sat} - p \right), \tag{18}$$

where C_{evap} is an empirical coefficient (= 0.001 in the investigation case). In the HK3 formulation the temperature discontinuity at the interface was considered, i.e.

$$\dot{\Gamma} = \frac{A_i\beta}{\sqrt{2\pi RT_{sat}}} \left(\frac{0.195\rho k + p_{sat}}{\sqrt{T_l}} - \frac{p}{\sqrt{T_{sat}}}\right).$$
(19)

⁸⁰² The value of 0.1 was used for the accommodation coefficient β .

Figures 5 (a) and (b) display the comparison of the numerical predictions of transient pressure and void fraction to experimental data. One can see that all the models have difficulty in capturing the flashing-inception, but the PPCM model based on the H-K equation gives overall better results compared to the HRM model.

Liao and Lucas [1] investigated the same case with the TPCM model in 808 ANSYS CFX. Apart from the different phase change model, they accounted for 809 the interphase slip velocity using the two-fluid model. A constant value of 1.0 810 mm was assumed for the bubble diameter, but the interfacial area density was 811 allowed to increase with the bubble number density as a result of phase change. 812 The comparison of the simulation results with those from [156] and experimental 813 data is shown in Figure 6. As expected, a better agreement was achieved by 814 using the TPCM model at the early stage of blowdown. The pressure undershoot 815 at the very beginning was captured well, which evidences the importance of 816



Figure 5: Edwards pipe simulation results from [156]: (a) pressure at P7 (b) void fraction at P4



Figure 6: Edwards pipe simulation results from [1]: (a) pressure at P7 (b) void fraction at P4

^{\$17} thermal non-equilibrium at this stage.

818 3.3. Flashing-induced instability (FII)

As discussed in the previous section, the FII problem concerning nuclear safety analysis has been investigated intensively with experiments and system codes, whereas CFD simulations are scarce. The challenges comprise highamplitude high-frequency waves, large geometry sizes and lack of CFD-grade experimental data. Liao et al. [1, 161, 162] presented CFD studies on the flashing and FII phenomenon observed at two test facilities, i.e. the AREVA INKA test facility [69] and the TUD GENEVA facility [78]. Both of them are down-



Figure 7: (a) KERENATM CCC system, (b) INKA riser [69, 161], (c) GENEVA riser [78, 162]

scale models of the containment cooling condenser (CCC) of the KERENA $^{\rm TM}$ 826 reactor, whose function and principle is sketched in Figure 7 (a). In case of 827 containment overpressure, steam condensed on the surface of the CCC tubes 828 and the heat is transported by the cooling water inside the tubes via the riser 829 to SSPV. In the INKA test facility, two sets of CCC were constructed and the 830 riser connecting CCC1 and CCC2 with SSPV comprises of vertical and sloped 831 pipes, see Figure 7 (b), while the GENEVA riser is a single straight pipe, which 832 is much longer as shown in Figure 7 (c). 833

Both simulations [1, 162] were performed with the two-fluid model in AN-SYS CFX, and the computational domain was restricted to the riser for high efficiency. The liquid and vapor phases were assumed in pressure equilibrium, and the TPCM was activated for interphase mass transfer. Bubbles have a spherical shape and the number density was prescribed as a constant value ($N_b = 5 \times 10^4$). Single-phase inlet was assumed, and the boundary conditions such as inlet mass flow rate, liquid temperature and outlet pressure were defined according to the



Figure 8: Comparison between simulation and measurement of pressure and temperature fluctuation in the INKA riser [1] (a) Pressure at CCC1, (b) Temperature at outlet

measurements. Figure 8 presents cross-section averaged pressure and tempera-841 ture transients inside the INKA riser, which conform well to the experimental 842 results. The simulation showed that the onset of flashing occurs at the highest 843 point of the domain due to low hydrostatic pressure, i.e. the top wall at the 844 outlet, and then propagated downward to the inlets. Separated and dispersed 84 flow was developed in the sloped and vertical pipe, respectively, and instability 846 waves were observed at the interface, see Figure 9. As the pressure recovered 847 the steam disappeared from bottom to top of the domain. 848

In order to reflect the non-uniform distribution of vapor bubbles at the cross 849 section of the pipe, needle-shaped conductivity probes were installed in the cen-850 tral and the peripheral region (about 2/3 of the inner diameter) at the GENEVA 851 test facility. Liao et al. [162] compared the local void fraction obtained numer-852 ically and experimentally, which discovered substantial difference. As shown 853 in Figure 10 the onset of flashing was delayed in the simulation. For example, 854 according to the experiment at z=3.99 m bubbles appear at the pipe center 855 before t = 20 s. On the other hand, the simulation gives non-zero void frac-856 tion after t = 50 s. Furthermore, the void fraction in the near-wall region is 857 under-predicted, see Figure 10 (b) and 10 (d). This discrepancy is partly caused 858 by the inaccurate prediction of bubble size, since non-drag forces representing 859 the lateral movement of bubbles depend on it directly. The assumption of a 860



Figure 9: Steam distribution in the INKA riser [161]

constant bubble number density deviates from the reality, leading to a uniform local bubble size, which is either smaller or larger than the real mean value. In this case, it might be over-predicted, since the bubbles are accumulated in the pipe center due to the effect of lift force. Nevertheless, both simulation and experiment evidenced that the flashing was initiated earlier at the pipe center than the periphery. Good agreement on the central void fraction was achieved at z = 4.99 m (see Figure 10 (c)).

868 3.4. Pressure relief transient

As shown in previous examples, flashing flows represent heterogeneous mix-869 ture of liquid and gas with void fraction ranging from zero to one. Reliable pre-870 diction of local phase distribution with the CFD tool represents still a challenge 871 relative to the cross-section averaged parameters such as pressure and tempera-872 ture. To improve the simulation results, it is of prime importance to reproduce 873 the bubble size change appropriately with the model, although equivalent ef-874 forts are needed in modelling of bubble forces, interphase heat transfer as well as 875 two-phase turbulence. For the purpose of model development, high-resolution 876 high-quality experimental data are valuable. Lucas et al. [163] presented exper-877 iments on flash evaporation in an 8 m long vertical pipe with an inner diameter 878



Figure 10: Comparison between simulation and measurement of local vapor void fraction inside the riser [162] (a) pipe center, z=3.99 m (b) 2/3 of the inner diameter, z=3.99 m (c) pipe center, z=4.99 m (d) 2/3 of the inner diameter, z=4.99 m



Figure 11: Pressure relief experiments at the TOPFLOW facility [163]

of 195.3 mm, carried out at the TOPFLOW facility. The phase change was 879 induced by depressurization of the pipe from 1, 2, 4 and 6.5 MPa. The pres-880 sure relief transient and evaporation process was investigated for circulating and 881 stagnant water, respectively, each with a different blow-off valve opening/closing 882 procedure, see Figure 11. Detailed information on the structure of gas-liquid 883 interfaces including spatial and temporal void fraction, bubble size distribution 884 as well as gas velocities was obtained by using a pair of wire-mesh sensors. Mea-885 surements are available for different combinations of opening/closing speed and 886 maximum opening degrees of the valve, which are represented by the parameters 887 R, t1, t2 and t3 in Figure 11. The database is suitable for the development and 888 validation of CFD models. Liao et al. [147, 164] presented detailed CFD stud-889 ies on the TOPFLOW pressure relief test cases based on the two-fluid model 890 with thermal phase change. The main focus was put on evaluating methods for 891 estimation of bubble diameter and interfacial area density, which vary from as-892 suming a constant bubble diameter or number density to using a poly-dispersed 893 894 approach. The main findings are summarized as follows:

895 896 • Mono-disperse approaches fail in predicting the bubble size change and thus the lateral movement of bubbles.



Figure 12: Comparison between simulated and measured radial void fraction profile at (a) t = 37 s, (b) t = 49 s, (c) t = 55 s, (d) t = 67 s

- The prescribed value for bubble diameter or number density affects the onset of flashing as well the evaporation rate in the simulation. A too large bubble diameter fails to trigger the phase change, while a too small one initiates it too early.
- The contribution of wall and bulk nucleation decreases and increases respectively with the pressure level.
- The poly-disperse approach with appropriate closures for bubble nucleation, coalescence and breakup improves the simulation results considerably. Radial void fraction and bubble size distribution are well captured as shown in Figures 12 and 13.
- Above CFD simulations of flashing flows are summarized in Table 3. They mainly differ in whether the velocity difference between phases is considered or



Figure 13: Comparison between simulated and measured radial void fraction profile at (a) t = 37 s, (b) t = 49 s, (c) t = 55 s, (d) t = 67 s

- ⁹⁰⁹ not (mixture or two-fluid model), what kind of phase change models (TPCM,
- ₉₁₀ PPCM, HRM or HEM) are adopted, and how to determine the interfacial area
- g11 density (constant N_B , d_B , variable N_B or poly-dispersity).

References and code	Numerical models and assumptions	Experiment
[35]	• homogeneous mixture model	BNL nozzle [26]
ANSYS CFX 4.2	• TPCM	
	• vapor at saturation	
	• transport equation for N_B	
	• wall nucleation considered	
[37]	• two-fluid model	BNL nozzle [26]
ANSYS FLUENT	• non-drag forces neglected	
	• TPCM	
	• interface at saturation	
	• heat transfer on vapor side neglected	
	• transport equation for N_B	
	• wall nucleation considered	
[39]	• two-fluid model	BNL nozzle [26]
ANSYS CFX 15.0	• drag and non-drag forces considered	
	• TPCM	
	• vapor and interface at saturation	
	• transport equation for N_B	
	• wall and bulk nucleation considered	
[40]	• two-fluid model	BNL nozzle [26]
ANSYS CFX 15.0	• drag and non-drag forces considered	
	• TPCM	
	• vapor and interface at saturation	
	• prescribed value N_B	
[145]	• two-fluid model	Moby Dick nozzle [146]
NEPTUNE_CFD	• drag and added mass force considered	
	• TPCM	

• vapor and interface at saturation• vapor and interface at saturation• prescribed value für d_B • wall nucleation considered as a mass source[36]• homogeneous mixture modelBNL nozzle [26]ANSYS FLUENT 6.1• PPCM based on the R-P equationISTF SGTR [151][150]• homogeneous mixture modelBNL nozzle [26]ANSYS FLUENT 12.0.16• PPCM based on the R-P equationLSTF SGTR [151][38]• homogeneous mixture modelBNL nozzle [26]• PPCM based on the H-K equationENL nozzle [26][41]• homogeneous mixture modelBNL nozzle [26]• slip model• PPCM based on the H-K equationENL nozzle [26][139]• homogeneous mixture modelBNL nozzle [26]in-house code• TPCM modelENL nozzle [26]in-house code• PPCM based on the H-K equationENL nozzle [26][3]• homogeneous mixture modelpipe flow [153, 154]OpenFOAM• relaxation model (HRM)Interface af groces[155]• two-fluid modelMoby Dick nozzle [146]NEPTUNE_CFD• very large drag forces• DEM model[159, 160]• two-fluid modelSG FWLB accidentANSYS CFX• non-drag neglected• TPCM model[156]• homogeneous mixture modelMoby Dick nozzle [146]ANSYS FLUENT• PPCM based on the R-P equation"Reitz" nozzle [146]			1
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• compared with the HEM, HRM model		$\bullet~$ compared with the HEM, HRM model	
[1] • two-fluid model "Edwards" pipe [42]	[1]	• two-fluid model	"Edwards" pipe [42]
ANSYS CFX 15.0 • TPCM INKA FII [69]	ANSYS CFX 15.0	• TPCM	INKA FII [69]

	• drag and non-drag cosidered	
	• prescribed value for d_B or N_B	
[162]	• two-fluid model	GENEVA FII [78]
ANSYS CFX 18.0	• TPCM	
	• drag and non-drag cosidered	
	• prescribed value for N_B	
[162]	• two-fluid model	TOPFLOW [163]
ANSYS CFX 18.2	• TPCM	
	• drag and non-drag cosidered	
	• population balance model	
	• wall and bulk nucleation considered	
	• coalescence and breakup considered	

Table 3: Summary of CFD studies on flashing flows

912 4. Conclusion

Although the numerical methods and models that have been used for analysis of flashing phenomena differ largely, there is some consensus concerning
following points:

In most cases, it is necessary to account for interfacial slip appropriately
 by using the two-fluid model.

Non-equilibrium phase change model is more general than the relaxation
 and equilibrium model. Thermal phase change model is superior to pressure phase change model, when thermal non-equilibrium effects are significant.

• Convection has a considerable contribution to the interfacial heat transfer in flashing flow, and conduction is dominant only in a short time after nucleation. • Appropriate modelling of bubble size and interfacial area density is crucial in modelling the interphase transfer. Taking into account the polydispersity is recommended by several researchers.

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• It is difficult to reproduce the lateral motion of bubbles, where non-drag forces play an important role in the interphase momementum transfer.

The prime challenges in CFD simulation of flashing flows arise from choosing ap-930 propriate closure models for interphase transfer, bubble dynamics (nucleation, 931 coalescence and breakup) as well two-phase turbulence. Further efforts regard-932 ing model improvement and data acquisition are required. Although tempera-933 ture difference is deemed to be the predominant driving force for phase change 934 in flashing situations, the effect of pressure difference might be substantial at the 935 inception, in particular at a large pressure undershoot. In most of the simula-936 tions, either pressure difference or temperature difference was neglected. There 937 is insufficient discussion on how to combine the two driving forces for phase 938 change properly. At high void fractions, the flow regime deviates widely from 939 bubbly flow, whereas the assumption of spherical bubbles were made in the ma-940 jority of works. Extending a multi-scale multi-field approach, for example the 941 GENTOP model proposed by Hänsch et al. [165], to handle different bubble 942 shapes is of interest in the future. Höhne et al. [166] and Höhne and Lucas 943 [167] have demonstrated the application of this model for various boiling cases. 944

945 **Declarations of interest:** none.

946 References

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