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Application of a hybrid multiphase CFD approach to the simulation of gas–liquid flow at a trapezoid fixed valve for distillation trays

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Abstract

In the present contribution, we demonstrate the application of a hybrid multiphase CFD approach, which allows for simulating dispersed phases as well as resolved interfaces within an Eulerian framework, for the flow on distillation trays for the first time. The morphology adaptive multifield two–fluid model is exemplified for continuous gas–liquid flow on a generic tray setup with a single trapezoid fixed valve. Instead of fully resolving its geometry in the computational grid, the gas inlets are emulated by implementing mass and momentum sources that are applied to local cell zones. Different zone types in terms of volume and curtain area are tested and compared. The simulation results are verified with experimental data from a lab–scale test rig with air–water flow. Local phase fractions were measured using a conductivity sensor array. The comparison of simulated and experimental results reveals that the relevant time–averaged and transient flow characteristics can be predicted satisfactorily if at least an approximate representation of the valve’s geometry in the computational grid is given. However, local differences are observed among the simulated phase distributions due to the varying cell zone volume and hence maximum intensity of the injected momentum.

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Keywords: distillation tray, fixed valve, morphology adaptive multifield two-fluid model, local source terms, CFD

1. Introduction

The increasing energy supply from renewable sources demands a more flexible operation of separation columns. In this context, tray columns with fixed valves trays are increasingly considered for revamps and new apparatuses, since they cope well with enlarged over and partial load modes when compared to sieve trays, cf. Lockett (1986), Goedecke (2006). However, considering the vast number of valve types and possible arrangements as well as their almost unpredictable impact on the complex liquid-vapor flow, the tray design is a challenging task in practice. This applies particularly in view of the fact that most fixed valves feature directional vapor outlets that may be utilized to guide the flow and to counteract liquid maldistribution and recirculation for the purpose of attaining high separation efficiencies, cf. Bell and Solari (1974), Vishwakarma et al. (2018). Nevertheless, tray design is often based on experience or rule of thumb, cf. Kister (1990), and the corresponding knowledge is usually kept undisclosed in the companies. However, in the context of increasing computational power (Markov, 2014, Waldrop, 2016) for simulating complex flow phenomena along with advanced measurement techniques (Hampel et al., 2020) for experimental validation of the underlying models, the application of computational fluid dynamics (*CFD*) becomes increasingly attractive to support the design process. But since it is still not feasible to resolve all details of the two-phase flow in an industrial-scale facility without high performance computing, customized solutions are required for practical daily use. Therefore, we aim at developing a three-dimensional coarse-grid CFD approach that enables engineers to simulate the most relevant scales of two-phase flow scenarios on fixed valve trays at reasonable computational effort.

Two-phase flow on distillation trays appears in various forms and is usually categorized into five major flow regimes (bubble, froth, spray, cellular foam and emulsion regime, cf. Lockett (1986), Kister et al. (1992)), which are associated with characteristic spatio-temporal distributions of vapor and liquid. Additionally, gradual transitions can occur between these major regimes, cf. Dhulesia (1983), Kister et al. (1992), like for many other two-phase flow phenomena, e.g. pipe flow (Wiedemann et al. (2019)) or bubble columns

34 (Nedeltchev et al. (2020)). Since the actual form of appearance depends on
35 operating conditions, fluid properties and — quite significantly — on the
36 tray design, the phase distribution and the dynamics of the flow cannot be
37 fully anticipated in the design process already. Moreover, the coexistence of
38 different regimes and phase structures should be assumed for an unbiased
39 simulation. This means that liquid-dominated as well as gas-dominated
40 regions may be present along with dispersed structures of the respective ac-
41 companying phase. However, two modeling approaches, which focus either
42 on continuous-continuous or continuous-disperse interactions, are presently
43 well-established for the simulation of gas-liquid flows.

44 On the one hand, the Volume of Fluid (*VoF*) model is applied with the
45 aim of resolving interfacial structures that are larger than the computational
46 grid size, e.g. for two-phase flows with large-scale interfaces or in the field of
47 microfluidics. For that purpose, VoF uses a computationally efficient single-
48 field approach for handling the two fluids by a single set of mass and momen-
49 tum equations. Interfaces are represented by gradients of a so-called color
50 function indicating the phases, cf. e.g. Ho (2017), Wörner (2012). How-
51 ever, this approach is impractical for industrial-scale flows with dispersed
52 structures due to the exceptional computational effort arising from the re-
53 quirement to resolve the interfacial structures on the grid, see e.g. Malvin
54 et al. (2014) who attempted to simulate the two-phase flow in a 1.213 m i.d.
55 sieve tray column. The authors used cell sizes of $(5 \times 2 \times 2) \text{ mm}^3$ at least
56 in the active zone of the tray to resolve the most relevant scales resulting
57 already in 3.8×10^6 computational cells when only accounting for half of the
58 actual domain by applying a symmetry boundary condition (*BC*). The latter
59 simplification is, however, not fully appropriate for assessing highly turbulent
60 three-dimensional flow fields on trays, cf. Jiang et al. (2012). Nevertheless,
61 the VoF model can be the method of choice for detailed investigations of the
62 flow through and around single valves. Alizadehdakhel et al. (2009) used the
63 VoF model for evaluating different geometric versions of a single float valve
64 in a small-diameter column. By assuming a fixed position of the valve and
65 resolving its full geometry in the grid, the authors were able to assess geom-
66 etry modifications by comparing the simulated gas distribution, interfacial
67 area and pressure drop.

68 On the other hand, two-phase flows can be treated with the so-called
69 Eulerian-Eulerian or Two-Fluid Model (*TFM*). Here, the two fluids are in-
70 terpreted as fully interpenetrating continua assuming that one fluid is dis-
71 persed in the other one, e.g. dispersed gas bubbles in a continuous liquid

72 phase. In the TFM approach, governing equations for the conservation of
 73 mass and momentum are established in a phase fraction weighted manner and
 74 are solved for both phases, cf. Ishii and Hibiki (2011). Since dispersed struc-
 75 tures are not resolved in the computational grid, submodels are formulated
 76 to describe the interfacial momentum coupling to account for unresolved in-
 77 terfacial forces like drag, lift, virtual mass etc. Due to the concurring nature
 78 of the bubble and froth regime on column trays, the vast majority of sim-
 79 ulation studies in this field makes use of the TFM, cf. Vishwakarma et al.
 80 (2018). Table 1 summarizes recent studies on TFM simulations of two-phase
 81 flows on trays with fixed and/or push valves.

Table 1: Literature on TFM simulation of two-phase flow on valve trays

reference	column i.d.	tray specifications	cell number
Zarei et al. (2009)	1.213 m	171 Mini V-Grid valves	$\approx 4.0 \times 10^5$ (half domain with symmetry BC)
Jiang et al. (2012)	0.574 m	10 triangularly shaped fixed valves	$\approx 5.1 \times 10^5$ (half domain with symmetry BC)
Li et al. (2014a)	0.570 m	sieve tray with 8 mm holes and 28 push valves	$\approx 7.3 \times 10^5$
Li et al. (2014b)	0.540 m	10 fixed valves	$\approx 1.5 \times 10^6$ (half domain with symmetry BC)
Zhao et al. (2018)	0.500 m	9 fixed valves with a push valve and 7 mm holes on top	$\approx 7.0 \times 10^5$ (half domain with symmetry BC)

82 Only Zarei et al. (2009) performed steady-state simulations directly, while
 83 the majority of studies considered the transient nature of the two-phase flow
 84 to derive temporally averaged distributions of hold-up and liquid velocity.
 85 Jiang et al. (2012) investigated the flow on a tray, in which the main openings
 86 of the fixed valves were either oriented in the direction of the main liquid flow
 87 or reversely. Li et al. (2014a) studied liquid velocities and hold-up distribu-
 88 tion on a sieve tray with push valves. The circular holes of the sieve were
 89 approximated by squares due to applying a structured Cartesian grid. The
 90 simulations of Li et al. (2014b) focused on the flow evolving from a particular
 91 fixed valve design with additional outlets in the valve cover providing an ex-
 92 tra pushing effect to the liquid phase. Similarly, Zhao et al. (2018) used the
 93 TFM to study the flow on a tray with comparably large fixed valves of 80 mm
 94 length with an additional push valve and sieve-like holes in the cover. For
 95 meshing this complex geometry cell sizes down to 2 mm were used locally at

96 the valves. With regard to modeling the unresolved interfacial drag between
97 liquid and the bubble swarm all of the above mentioned studies followed the
98 approach of van Baten and Krishna (2000) and used empirical correlations
99 for estimating the average gas fraction in the froth zone that is used to calcu-
100 late the local slip velocity. However, while e.g. van Baten and Krishna (2000)
101 and Gesit et al. (2003) applied a well-established literature correlation for
102 their sieve tray simulations, Jiang et al. (2012), Li et al. (2014a,b), Zhao
103 et al. (2018) simply fitted new coefficients for this correlation by regression
104 analysis based on their own experimental data. The obtained coefficients
105 vary significantly across these studies. Thus, no universal validity can be at-
106 tested. Furthermore, drag at large-scale interfaces is not described properly
107 in this approach leading to inaccuracies, in particular for jetting gas inlets
108 on fixed valve trays as observed in the results of e.g. Jiang et al. (2012). In
109 this context only Li et al. (2014b) included a free surface model to counteract
110 diffusion of the resolved large-scale interface. However, an even more funda-
111 mental issue is that the standard TFM suffers from the fact that only one
112 fluid is dispersed in the other one (usually gas in liquid). Thus coexisting
113 regimes, like e.g. froth in the lower region and spray in the upper region of
114 the two-phase zone, cannot be captured accurately at the same time.

115 In summary, neither the VoF model nor the standard TFM allow for
116 capturing all flow morphologies observable on industrial-scale distillation
117 trays with acceptable computational burden. Therefore, it is desirable to
118 combine the advantages of both models within a hybrid approach, cf. Hänsch
119 et al. (2012), Frederix et al. (2021), Colombo et al. (2022). Recently, Meller
120 et al. (2021) proposed a morphology adaptive multifield two-fluid model
121 that is capable of handling both types of interfacial structures — those being
122 smaller than the computational grid size, as well as those, which are larger —
123 within in a single computational framework. More precisely, four numerical
124 phases (continuous gas, continuous liquid, dispersed gas, dispersed liquid) can
125 be considered here and an individual treatment of their interactions is applied
126 with appropriate models in a VoF-like or TFM-like manner depending on
127 the local composition of the phase mixture, i.e. the local flow morphology. In
128 principle, this hybrid approach enables the prediction of two-phase flow on
129 distillation trays without prior assumptions of the actual flow structure. The
130 public source code of this morphology-adaptive multifield two-fluid model is
131 provided by Schlegel et al. (2022).

132 The present contribution describes the application of Meller’s hybrid
133 model (Meller et al., 2021) for the gas-liquid flow on a generic distillation

134 tray with a single fixed valve. For the sake of reduced computational effort
135 along with the objective of using coarse grids for industrial-scale simula-
136 tions in future, local mass and momentum sources are used to mimic the
137 gas injection through the valve instead of resolving its full geometry with
138 the computational grid. While our previous contribution (Wiedemann et al.,
139 2022) verified the applicability of this approach and revealed that oscillat-
140 ing sources are needed to properly reproduce the dynamics of the gas in-
141 jection, the present study focuses on the geometrical representation of the
142 valve. Therefore, different sizes of the cell zones, in which the gas is in-
143 jected, are investigated with respect to the resulting phase distribution near
144 the valve. Temporally averaged phase contours and liquid velocity fields as
145 well as transient characteristics are compared among the different cases and
146 against experimental data.

147 2. Modeling approach

148 The applied morphology adaptive modeling framework is able to han-
149 dle dispersed as well as resolved interfacial structures, which may coexist in
150 the computational domain, with the same set of equations, cf. Meller et al.
151 (2021). It is essentially based on an Eulerian multifield two-fluid model,
152 in which phase specific, ensemble averaged transport equations are formu-
153 lated. The governing equations for each numerical phase i are given by the
154 conservation of mass

$$\frac{\partial(\alpha_i \varrho_i)}{\partial t} + \nabla \cdot (\alpha_i \varrho_i \vec{v}_i) = \dot{m}_{i,S} \quad (1)$$

155 and momentum

$$\begin{aligned} & \frac{\partial(\alpha_i \varrho_i \vec{v}_i)}{\partial t} + \nabla \cdot (\alpha_i \varrho_i \vec{v}_i \otimes \vec{v}_i) \\ & = -\alpha_i \nabla p + \nabla \cdot (2\alpha_i \mu_i \bar{\bar{S}}_i) + \alpha_i \varrho_i \vec{g} + \vec{f}_i^\sigma + \vec{f}_i^{MT} + \vec{f}_{i,S}. \end{aligned} \quad (2)$$

156 Here, α_i denotes the volumetric phase fraction of each phase i adding up
157 to unity across all phases. ϱ_i and \vec{v}_i are the density and velocity of phase i ,
158 respectively. The pressure p is shared among all phases. μ_i is the effective dy-
159 namic viscosity, $\bar{\bar{S}}_i$ the strain rate tensor and \vec{g} the gravitational acceleration.

160 \vec{f}_i^σ represents the surface tension force, which is only applied to interfaces of
161 continuous–continuous phase pairs and modeled according to Brackbill et al.
162 (1992). \vec{f}_i^{MT} summarizes the interfacial momentum transfer. For unresolved
163 momentum transfer in continuous–disperse phase pairs \vec{f}_i^{MT} includes closure
164 models for drag, lift, virtual mass, turbulent dispersion and wall lubrication,
165 which are chosen according to Liao et al. (2019). In contrast, for resolved in-
166 terfaces of continuous–continuous phase pairs \vec{f}_i^{MT} includes drag only. In this
167 case, the model of Štrubelj and Tiselj (2011) is applied in connection with a
168 very low interfacial relaxation time, which ensures a no–slip condition at the
169 interface. The closure models for the interfacial momentum transfer \vec{f}_i^{MT} are
170 immutably selected for pairs of either continuous–continuous or continuous–
171 dispersed phases based on the fixed roles of the individual phases, i.e. each
172 individual phase is designated to be either of dispersed or of continuous mor-
173 phology, cf. Meller et al. (2021). However, as the present study focuses on
174 the influence of injecting continuous gas into the continuous liquid phase,
175 dispersed phases are neglected here. In order to account for gas injection
176 through the fixed valve additional sources for mass $\dot{m}_{i,S}$ and momentum $\vec{f}_{i,S}$
177 are considered in equations (1) and (2), respectively. Note that these are
178 applied locally in the continuous gas phase only, see section 3.2.

179 3. Simulation setup

180 3.1. Experimental basis

181 The computational setup is based on experimental investigations that
182 were performed using the facility shown in figure 1. The experimental facility
183 is made of PMMA and features a rectangular tray of 670 mm length (x -
184 direction = liquid inlet to weir) and 400 mm width (y -direction). The facility
185 is 530 mm high (z -direction) and the top is open to the atmosphere. Both
186 downcomer clearance and weir height were fixed to 50 mm. A single R-
187 FV trapezoid standard fixed valve from *Raschig* (dimensions are depicted in
188 figure 1) with a lift height of 7 mm was installed at the center of the tray,
189 which is defined as the origin of coordinates (x, y, z) .

190 The facility was operated with liquid water (l) and gaseous air (g) at
191 ambient conditions. The liquid flow was driven by a centrifugal pump and
192 measured by a magnetic–inductive flow meter in the feed pipe. A flow rate
193 of $\dot{V}_l = 15.25 \text{ m}^3/\text{h}$ was adjusted and kept constant during the experiments,
194 which corresponds to a weir load of $38.1 \text{ m}^3/(\text{h m})$ and an average inlet ve-
195 locity of $v_{l,x} = 0.21 \text{ m/s}$. Gas was supplied by the compressed air line of

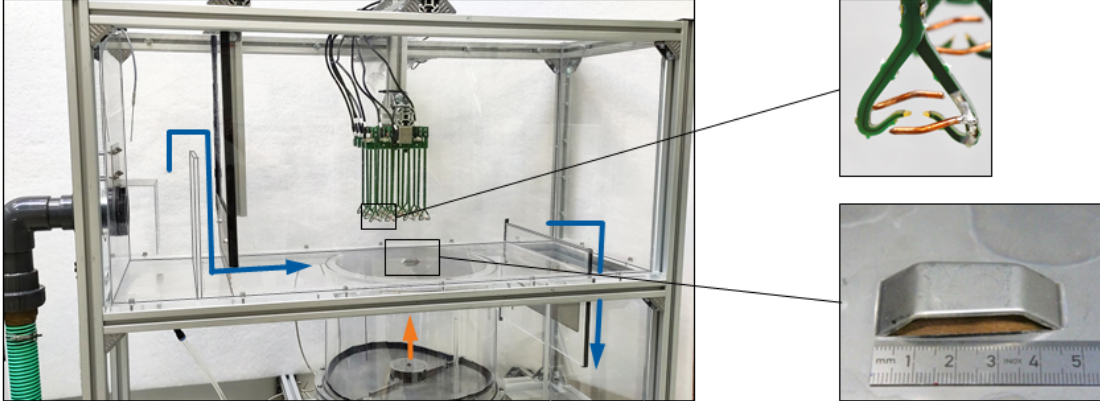


Figure 1: Experimental facility with investigated R-FV fixed valve and conductivity sensor array. Blue and orange arrows indicate flow of liquid and gas, respectively.

196 the laboratory and adjusted by a mass flow controller. The gas entered the
 197 DN400 cylindrical vessel below the tray, see figure 1. After passing a baffle
 198 plate to ensure homogeneous distribution in the vessel, the gas passes the
 199 centered valve on top of the vessel. Taking into account the local tempera-
 200 ture and pressure inside the vessel, a local gas flow rate of $\dot{V}_g = 3271/\text{min}$ was
 201 obtained in the present experiments. According to the curtain area (CA) of
 202 the valve, this yields an average gas velocity of $v_{g,CA} = 11.7 \text{ m/s}$ or in terms
 203 of the F-factor $F_{CA} = 12.9 \text{ Pa}^{0.5}$. It should be noted that F_{CA} corresponds
 204 to the hole F-factor and not the F-factor being based on the active area,
 205 which cannot be defined in a meaningful manner for the present setup.

206 During the experiments the phase distribution around the valve was mea-
 207 sured using the conductivity sensor array shown in figure 1. The sensor is a
 208 slightly modified version of the one proposed by Vishwakarma et al. (2021)
 209 and is based on the operating principle of a wire-mesh sensor, cf. Prasser
 210 et al. (1998). The present sensor is characterized by a new probe tip design
 211 featuring additional local shielding and an improved shape to prevent droplet
 212 accumulation in the tip region when operating in the spray zone. Local phase
 213 fractions were measured with a frequency of 2500 Hz for 60 s of flow time dur-
 214 ing steady-state operation at various positions around the valve. After time-
 215 averaging of the individual data sets the results were merged to form a matrix
 216 with $8 \times 8 \times 7$ points with a spacing of $(\Delta x, \Delta y, \Delta z) = (40, 40, 25) \text{ mm}$ that
 217 represents the three-dimensional mean phase fraction distribution. This ma-

218 trix serves as basis for interpolating phase contours for the comparison with
219 simulation results.

220 3.2. Computational setup

221 The experimental facility is captured in the computational setup with its
222 original dimensions as shown in figure 2. However, only 400 mm height are
223 considered above the tray to reduce computational effort.

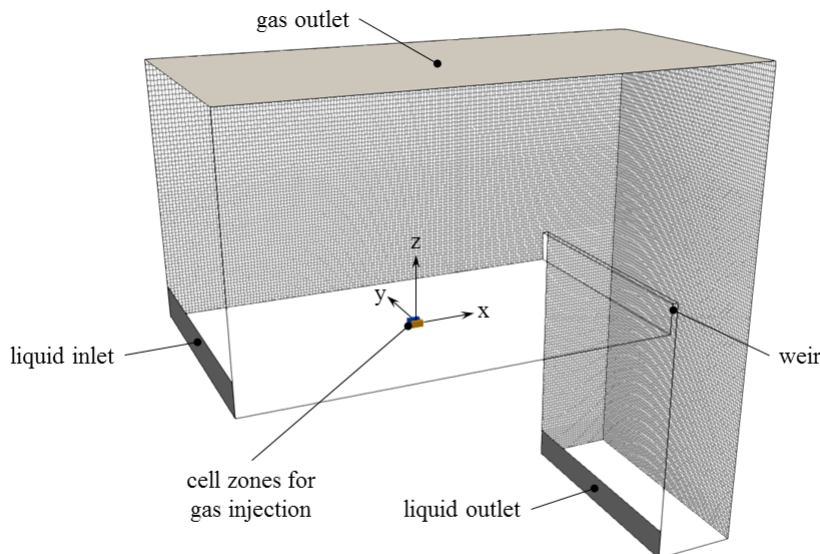


Figure 2: Computational domain with boundary conditions and cell zones for the implementation of local sources

224 The boundary conditions comprise no-slip at all solid walls, i.e. the tray,
225 all side walls as well as the weir. A homogeneous velocity is assumed at
226 the inlet of the liquid phase, which corresponds to the average experimental
227 value of $v_{l,x} = 0.21$ m/s. Such a flat velocity profile has also been used by
228 other authors (cf. Jiang et al., 2012, Li et al., 2014b) and is reasonable when
229 considering the highly turbulent flow in the preceding downcomer, cf. Mehta
230 et al. (1998). For the liquid outlet we apply a so-called matched flow rate
231 condition, which regulates the outlet velocity according to the flow rate at
232 the inlet. In this way, a steady operation point with constant filling level in
233 the downcomer is obtained. The top of the domain is modeled as a stan-
234 dard Neumann type boundary for outflow with optional backflow for the
235 gas phase. For the injection of gas through the curtain area of the valve,

236 the concept of Wiedemann et al. (2022) is applied, i.e. the gas inlets are
 237 mimicked by implementing mass and momentum sources that are applied to
 238 local cell zones exclusively (see figure 2). As shown by Wiedemann et al.
 239 (2022), dynamic gas injection is required to account for proper dynamics of
 240 bubble/jet detachment at the valve, since the complex interaction with the
 241 compressible gas volume below is not captured inherently in a single tray
 242 simulation. Hence, a sinusoidal gas injection is selected in the present study
 243 and the source terms for equations (1) and (2) read

$$\dot{m}_{g,S}(t) = \frac{\dot{V}_g \rho_g}{2} [\sin(2\pi f_d t) + 1] \quad (3)$$

244 and

$$\vec{f}_{g,S}(t) = \dot{m}_{g,S}(t) v_{g,CA} [\sin(2\pi f_d t) + 1] \cdot \vec{n}_{CA} , \quad (4)$$

245 respectively. Here, f_d denotes the dominant frequency that was deter-
 246 mined from the experimental data by spectral analysis and is associated
 247 with the gas detachment frequency. For the operating conditions described
 248 in section 3.1 the dominant frequency is $f_d = 7.32$ Hz. The factor 1/2 in
 249 equation (3) stems from the fact that the R-FV fixed valve is symmetrical
 250 with respect to $y = 0$, see figure 1, and the total gas flow rate is assumed to
 251 split equally to the left and right side of the valve. Accordingly, an individ-
 252 ual cell zone is considered for each side of the valve. At the same time, this
 253 allows for modeling the directional gas injection by means of equation (4),
 254 in which \vec{n}_{CA} denotes the face normal vector of the respective curtain area.
 255 Due to symmetry solely the sign of the y -component of \vec{n}_{CA} differs between
 256 the left and right side of the valve.

257 For the application of equation (3) it must be considered that (in each
 258 time step) the mass flow rate is equally distributed among all grid cells of
 259 the selected cell zone. Since the possibilities of representing the valve's ge-
 260 ometry by means of cell zones are limited due to the coarse resolution of the
 261 computational grid, different scenarios are investigated here, cf. table 2.

262 All cases are restricted by a minimum lift height of 10 mm and hence
 263 overestimate the actual lift height of the valve. While cell zone type a)
 264 approximately recovers the real length of the valve, type b) gives the best
 265 representation with respect to the curtain area, which is approximated by

Table 2: Overview of investigated cases with different representation of the valve’s geometry by cell zones

cell size	$(9.85 \times 10 \times 10) \text{ mm}^3$		$(10 \times 10 \times 10) \text{ mm}^3$
cell zone type	a)	b)	c)
lift height/mm	10	10	10
length/mm	39.4	19.7	10
total curtain area/mm ²	788	394	200
total volume/mm ³	7882	3941	2000

266 the outer planes in $\pm y$ -direction here. Cell zone type c) is equivalent to the
 267 extreme case of a point-like source. Note that the total volume of the zone
 268 influences the maximum local intensity of the mass flow rate and hence of the
 269 momentum source, while the shape of the curtain area affects the mapping
 270 of the region of interest.

271 The investigated scenarios resulted in a total number of 1.36×10^5 com-
 272 putational cells. A time step size of $\Delta t = 5.0 \times 10^{-5} \text{ s}$ provided a stable
 273 convergence behavior for the numerical solution. Details on the numerical
 274 solution procedure can be found elsewhere, see Meller et al. (2021).

275 As a transient process is simulated, the evaluation of the results needs to
 276 consider start-up effects that are neglected prior to analyzing field variables.
 277 In order to speed up the start-up process in the simulations, the tray region
 278 between inlet and weir as well as the downcomer are initialized with liquid,
 279 i.e. $\alpha_l = 1$. Previous investigations on the treated single-valve arrangement
 280 showed that 5 s of start-up period were sufficient under these conditions,
 281 cf. Wiedemann et al. (2022). Moreover, this period represents about 1.5
 282 times the average residence time of liquid on the tray and about 36 events of
 283 bubble/jet detachment in the region of interest. Similar values of (4...8) s
 284 are reported in the literature on simulations of full trays, cf. Jiang et al.
 285 (2012), Li et al. (2014a,b). With regard to the subsequent period to be an-
 286 alyzed, 5 s and 10 s were chosen by Jiang et al. (2012) and Li et al. (2014a),
 287 respectively. Although our previous study (Wiedemann et al., 2022) revealed
 288 almost independent results for an evaluation period of 5 s, too, 10 s are cho-

289 sen conservatively in the present study for the sake of statistical reliability.
290 Hence, all results in section 4 refer to a flow time of $t = (5 \dots 15)$ s.

291 4. Results and Discussion

292 4.1. Analysis of time-averaged phase distribution and liquid velocity

293 To evaluate the influence of gas injection through the different cell zone
294 types presented in table 2, the resulting distributions of time-averaged phase
295 fractions (holdup) are analyzed. In order to characterize the turbulent two-
296 phase froth zone on temporal average, contours at two levels of the time-
297 averaged gas phase fraction are chosen. The value of $\overline{\alpha}_g = 0.75$ is interpreted
298 as time-averaged interface between froth and pure gas, whereas $\overline{\alpha}_g = 0.25$
299 is treated as interface between froth and pure liquid. Qualitative differences
300 are already observed in figure 3 depicting the three-dimensional contours of
301 the investigated cases.

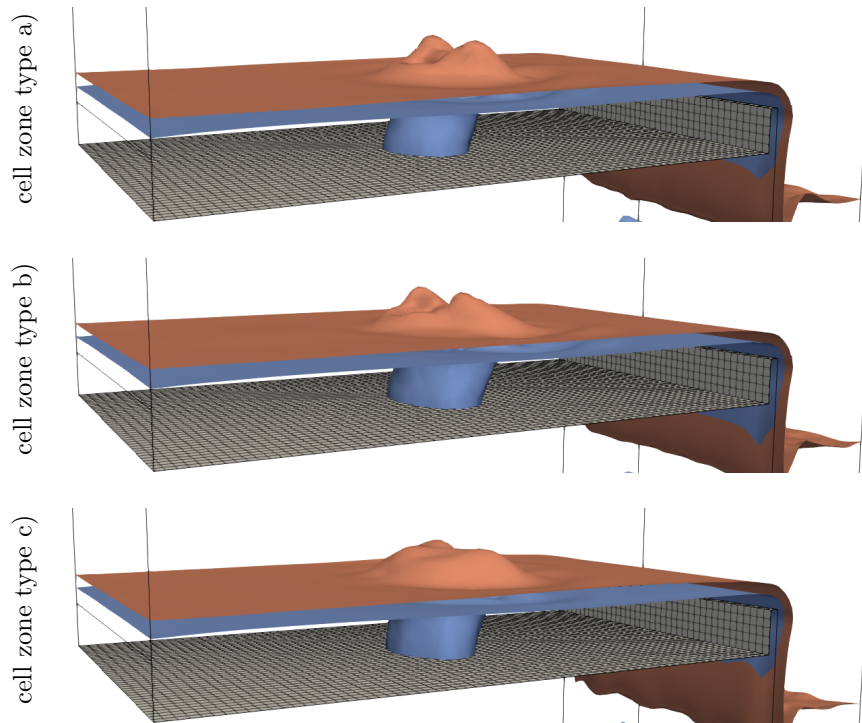


Figure 3: Contours of $\overline{\alpha}_g = 0.75$ (red) and $\overline{\alpha}_g = 0.25$ (blue) for the investigated cell zone types

302 The froth–liquid interface ($\overline{\alpha}_g = 0.25$) represented by the blue surface
 303 forms a hose connecting the tray in the region of the valve with the liquid
 304 surface. The girth of this froth hose is predicted to be smallest with the
 305 longest injection cell zone (type a) and largest with the intermediate zone
 306 length (type b). Due to the liquid flow, this froth structure is inclined to-
 307 wards the liquid downstream direction. That inclination is prominent when
 308 using long and intermediate injection cell zones, types a) and b), respectively.
 309 However, the short injection cell zone (type c) leads to a weaker inclination of
 310 the froth hose. Considering the froth–gas interface ($\overline{\alpha}_g = 0.75$) represented
 311 by the red surface, the different cell zone types reveal different qualitative
 312 behavior. While the short injection cell zone (type c) produces a flat hill el-
 313 evated from the free liquid surface, cell zone types a) and b) cause two sharp
 314 peaks. Presumably, those are pushed up by the two individual streams of
 315 gas originating from the two separated injection cell zones in the numerical
 316 setup. The results produced with the long and intermediate injection cell
 317 zones, types a) and b), respectively, appear to be qualitatively similar.

318 Detailed analysis and quantitative comparison are shown below for the
 319 lateral distribution near the valve. Since the injected gas contains a velocity
 320 component in positive x -direction and is further exposed to drag of the hor-
 321 izontal liquid flow, a slight displacement in positive x -direction is observed
 322 for the formed structures in the experiments and simulations. The analy-
 323 sis is hence carried out for two positions downstream of the valve, namely
 324 $x = 20$ mm and $x = 60$ mm, cf. figures 4 and 5.

325 Considering the liquid–froth interface ($\overline{\alpha}_g = 0.25$) at $x = 20$ mm in fig-
 326 ure 4 the long injection cell zone, type a), delivers the narrowest froth hose,
 327 which confirms the observation from the three–dimensional surfaces. This
 328 can be explained by the fact, that injecting a given mass flow rate into a
 329 larger volume, i.e. cell zone, results in a lower injection velocity and hence
 330 in a lower momentum injection compared to a smaller injection cell zone,
 331 such as types b) or c). That leads to a widening of the froth hose with the
 332 latter two types of injection zone. All types of injection zones reveal a wider
 333 froth hose compared to experimental observations. A feature, which is only
 334 predicted with the long injection zone (type a) is the presence of two large
 335 gas jets ($\overline{\alpha}_g = 0.75$) originating from the tray next to the locations of gas
 336 injection and reaching the altitude of the free liquid surface. An explanation
 337 for this phenomenon is the comparably low amount of injected momentum as
 338 described before for cell zone type a), which does not deliver enough energy
 339 to instantly break up larger gas structures as it is the case for injection zone

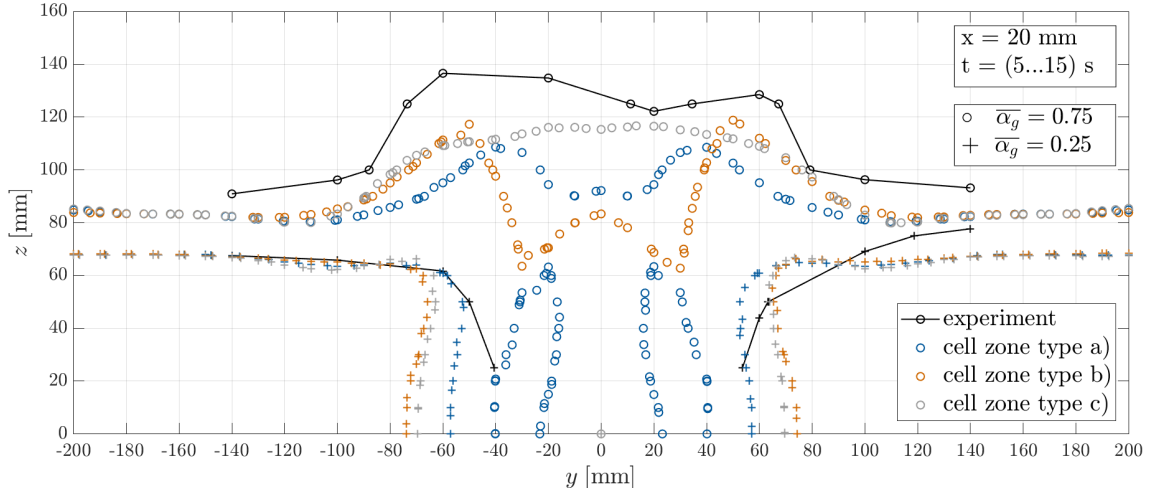


Figure 4: Comparison of time averaged phase distribution from simulation with different cell zones against experiment at $x = 20$ mm

340 types b) and c). Hence, with type a) injection cell zones the gas structures
 341 exist longer and, therefore, are more compact and hereby become visible as
 342 liquid–froth interface. The experimental data do not show such large–scale
 343 gas structures attached to the injection valves. However, jet formation and
 344 detachment were also observed visually in the experiments, but is not seen
 345 in the experimental data due to the coarse resolution of the sensor with a
 346 low number of grid points for the interpolation of the phase contour in this
 347 region. For the upper froth–gas interface ($\overline{\alpha}_g = 0.75$) the observations from
 348 the three–dimensional surfaces are confirmed as well, such that the double
 349 peak structure occurs for the long and intermediate injection zones, types a)
 350 and b), respectively, while the short injection zone (type c) delivers a flat
 351 hill. The experimental data show such a double peak structure which is
 352 much more shallow compared to the simulation results of cell zone types a)
 353 and b), while the absolute elevation of the froth–gas interface is measured
 354 to be slightly larger compared to the computational results for all injection
 355 zone types under investigation. In the results obtained with cell zone type b)
 356 a relatively deep cavity of the froth–gas interface is observed between both
 357 peaks, which is neither seen with the other injection zone types nor in the
 358 experiment. The lateral expansion of the upper froth contour is predicted
 359 reasonably well in all simulations. Further away from the region of gas in-
 360 jection, i.e. $y < -120$ mm and $y > 120$ mm, the levels of both liquid–froth

361 and froth–gas interfaces are insensitive to the choice of the cell zone type
 362 for gas injection. Therefore, a spatially limited influence of the zone type is
 363 attested. However, compared to experimental data the simulated interfaces
 364 are located slightly below the experimentally measured ones.

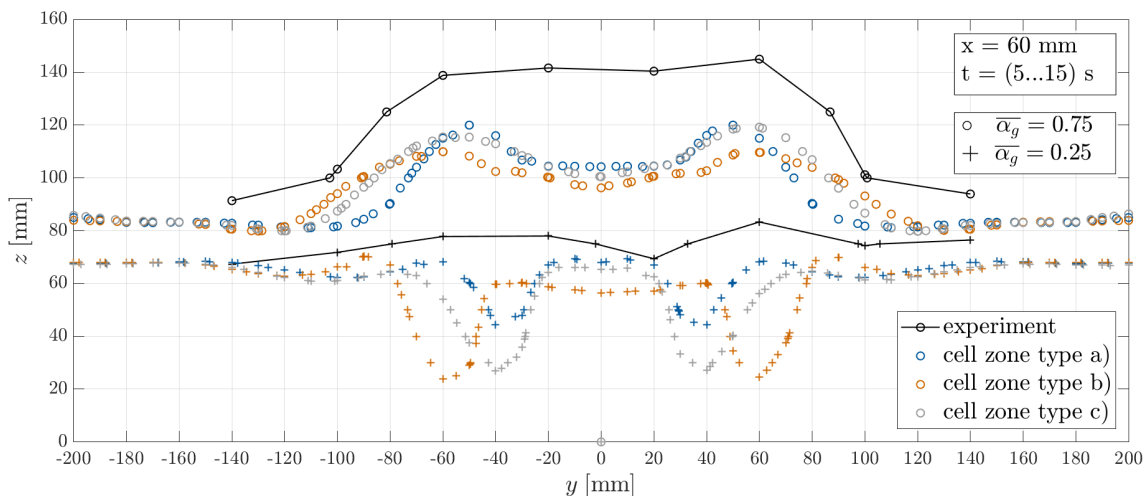


Figure 5: Comparison of time averaged phase distribution from simulation with different cell zones against experiment at $x = 60$ mm

365 At $x = 60$ mm (see figure 5) the different injection zone types reveal
 366 qualitatively similar results for the location of the time-averaged froth–gas
 367 interface ($\overline{\alpha}_g = 0.75$) showing two comparably flat peaks. However, the gra-
 368 dient of the interface height is predicted to be steeper with type a) injection
 369 zones compared to types b) and c). The elevation of the froth–gas interface
 370 measured in the experiment is, again, larger than in the simulation results
 371 and a flat hill structure is observed rather than a two peaks. Also shape
 372 and location of the liquid–froth interface ($\overline{\alpha}_g = 0.25$) are qualitatively simi-
 373 lar among all simulation setups showing two small cavities. The cavities are
 374 predicted to be similarly deep with cell zone types b) and c), while type a)
 375 results in more shallow structures here. The distance between those cavities
 376 are similarly small for cell zone types a) and c), while being larger for type b).
 377 The cavities cannot be observed in the experimental data.

378 In order to further evaluate the local effect of the different zone types,
 379 the time-averaged liquid velocity field is investigated on the horizontal plane
 380 $z = 5$ mm, i.e. in the lowest cell layer directly on the tray. In figure 6 results

381 are presented in terms of contours of velocity magnitude and vector fields for
 382 all three cell zone types studied.

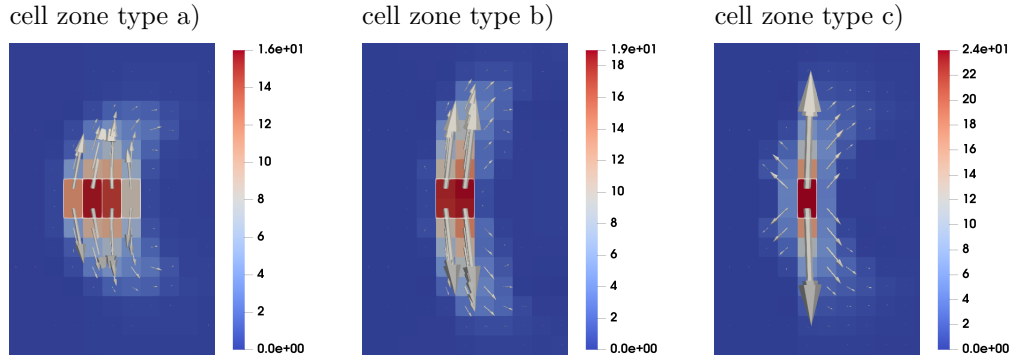


Figure 6: Contours and vectors of time-averaged liquid velocity in m/s at $z = 5$ mm above the tray (main liquid flow direction from left to right, the cell zone for gas injection is marked with white contours)

383 In accordance with the direction of gas injection through the valve, the
 384 liquid is accelerated in opposite lateral directions via gas-liquid momentum
 385 transfer in all cases. However, with increasing distance from the injection
 386 location the effect rapidly decays until the liquid flow appears completely
 387 unaffected after approximately (40...50) mm from the curtain area. Thus,
 388 the liquid flow is increasingly bent towards the downstream direction of the
 389 liquid background flow. According to the biggest length of injection zone
 390 type a) the affected region of laterally accelerated liquid is the longest among
 391 the investigated cases. The shorter the injection cell zones with types b) and
 392 c), the larger is the injection velocity due to the fixed injection gas flow rate.
 393 With cell zone type c) the maximum liquid velocity observed at $z = 5$ mm is
 394 roughly 50% larger than with type a). The injected gas locally displaces the
 395 liquid and for cell zone type c) this effect becomes so strong that a significant
 396 local backflow is observed in the upstream direction of the liquid background
 397 flow in front of the cell zone. This may also explain the smaller inclination of
 398 the liquid-froth interface ($\overline{\alpha}_g = 0.25$) in figure 3, which probably also leads to
 399 accumulating more liquid in the stagnation point to finally fill up the double-
 400 peak structure of $\overline{\alpha}_g = 0.75$ observed for type a) and b) in figure 4. However,
 401 due to the local concentration of the gas injection in cell zone type c) and
 402 the resulting large velocity gradients, the dissipation of kinetic energy is so
 403 strong that the liquid velocity quickly decreases with growing distance from
 404 the injection zone. Therefore, the pattern of the liquid velocity observed in

405 the horizontal plane close to the injection valve is quite similar to cell zone
406 types a) and b).

407 Overall, the qualitative behavior of the system is not excessively influ-
408 enced by the choice of the injection zone type, if the length of the cell zone
409 is not too short as present for type c). In the latter case, flow features such
410 as a slender froth hose or a double peak of the froth–gas interface cannot be
411 predicted in contrast to longer injection zone types a) and b). Finally, the
412 simulation with cell zone type a) provides the best fit with the experimental
413 data of gas injection through a single fixed valve. However, higher spatial
414 resolution of the experimental data is required in future to obtain more de-
415 tails of the gas–liquid interface and of the flow near the valve, such as gas
416 jets and bubbles.

417 *4.2. Analysis of transient phase fraction characteristics*

418 In addition to the analysis of the time–averaged phase distributions, the
419 transient behavior of the phase fraction is evaluated for two positions near
420 the valve. Here, the closest probe positions slightly downstream of the valve
421 at the lowest sensor elevation of $z = 25$ mm were selected, namely a left probe
422 at $(20, 20, 25)$ mm and a right probe at $(20, -20, 25)$ mm. For the analysis
423 a representative time span of 0.5 s is arbitrarily chosen from the full time
424 series. Figure 7 shows the temporal evolution of the measured and simulated
425 gas fractions.

426 The experimental time series show almost synchronously fluctuating gas
427 fractions between 0 and 1 in a square pulse fashion, which is attributed
428 to the almost simultaneous formation and detachment of large gas jets or
429 bubbles on both sides of the valve. As the dominant frequency of these
430 fluctuations is directly used in equations (3) and (4) without any time shift,
431 the simulated time series consequently predict similar dynamics. The reasons
432 for deviations on smaller time scale are twofold. Firstly, the superposition
433 with random effects in the real flow, e.g. small bubbles, and other frequencies
434 is not considered in the injection model. Secondly, the volume averaging
435 nature of CFD does not allow for a point–like data acquisition as done in the
436 experiment. The latter may also be the reason for not reaching pure liquid,
437 i.e. $\alpha_g = 0$, in the simulations.

438 With regard to the different cell zones for gas injection it can be observed
439 from figure 7 that type a) and b) yield an almost constantly repeated os-
440 cillation, while much more irregular amplitudes of α_g are obtained for the

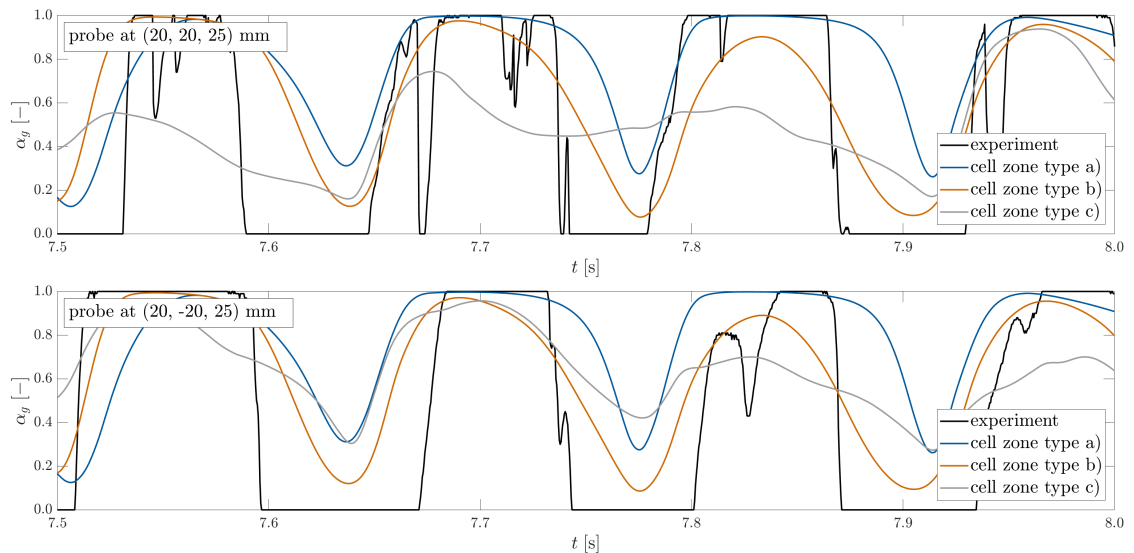


Figure 7: Temporal evolution of gas phase fraction on left (top) and right (bottom) side of the valve

441 point-like injection with cell zone type c). Moreover, notable differences be-
 442 tween the left and right side of the valve are seen for type c), whereas cell
 443 zone types a) and b) show a consistent course for both sides. The apparent
 444 differences in the duty cycle and also in the overall level between type a) and
 445 b) can be explained by the length of these cell zones. With respect to the
 446 x -coordinate the probe positions coincide with the downstream end of cell
 447 zone type a), but exhibit an offset for the intermediate cell zones of type b).
 448 Hence, the gas pulse replaces more liquid locally at the probe positions for
 449 type a) when compared to type b). In this way type a) also provides the
 450 experimentally observed feature of longer periods with $\alpha_g = 1$. On the other
 451 hand, however, the intermediate length of zone type b) provides higher mo-
 452 mentum during the injection (see also figure 6), which leads to faster passage
 453 of the detached gas and thus better agreement with the shorter experimen-
 454 tal duty cycle. Basically, the above argumentation applies also to cell zone
 455 type c), since lower gas fractions are observed at the probes (due to the
 456 much larger distance to the injection zone) and broader cycles are obtained
 457 according to the smaller influence of the momentum source in these points
 458 (see figure 6). However, an explanation for the irregular behavior cannot be
 459 given here.

460 When focusing on the abrupt changes between liquid and gas in the ex-
461 periments, only the long (type a) and intermediate (type b) cell zones provide
462 a reasonably steep increase of the gas fraction at the beginning of each pulse,
463 in particular, when taking volume averaging into account. However, the de-
464 cline part of the gas pulses is significantly flatter and does poorly agree
465 with the experimental results. A possible reason might be slow bubble de-
466 tachment, which could be attributed to the neglected but possibly present
467 z -component at the gas inlets, or to a deviating jet or bubble growth rate.
468 Nevertheless, against the background of coarse-grid simulations the applica-
469 tion of cell zone types a) and b) leads to a reasonable agreement with the
470 experimentally observed dynamics.

471 5. Conclusions

472 A morphology adaptive multifield two-fluid model was used to simulate
473 the two-phase flow on a generic distillation tray setup with a single trape-
474 zoid fixed valve. The valve was emulated by the implementation of local
475 mass and momentum sources in the gas phase. Different geometric represen-
476 tations of the valve were investigated in the form of varying size of the cell
477 zones for the gas injection. The comparison of the simulation results with
478 experimental phase fraction data from a conductivity sensor array showed
479 that the formation of the characteristic froth zone is basically accomplished
480 by all investigated cell zone types. However, local differences are observed
481 with respect to mapping the gas injection to the computational grid and due
482 to the resulting intensity of the momentum source. With regard to evalu-
483 ating the local dynamics of the two-phase flow, the relation between mesh
484 resolution, probe location and size of the gas injection zone plays a crucial
485 role for the analysis. From the present study it can be concluded that at least
486 an approximate representation of the valve's geometry in the computational
487 grid is necessary to properly predict the main characteristics. Point-like im-
488 plementations of the source terms did not provide reasonable agreement with
489 the experimental data regarding the dynamics.

490 Based on the current results, future investigations will focus using the full
491 capabilities of the hybrid model in terms of additionally considering dispersed
492 gas and liquid phases. Further, more complex valve geometries as well as
493 multiple valve arrangements need to be studied to transfer the approach to
494 industrial-scale distillation trays in the future.

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