

CFD modelling of R410A flow through an Expansion Valve using Equilibrium and Modified Relaxation Models

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Abstract

The two-phase flow of R410A refrigerant through an electronic expansion valve (EEV) is modelled using two models, the Homogeneous Equilibrium Model (HEM) and Homogeneous Relaxation Model (HRM) in a CFD numerical analysis. The reason for this is to take a step towards developing a more generic description of two-phase flow calculations. The EEV, applied in air-conditioning and refrigeration systems, was examined by measuring the mass flow rate of the refrigerant, the pressure and the temperature at the valve inlet, and the pressure at the outlet. The EEV was regulated using pulse width modulation; however, during the experiments the EEV was fully opened. Operation of the valve was carried out over a sub-cooling range of 3.8 to 7.7 K. The expansion process started from around 20 bar and ended within the pressure range of 6.8 to 11.5 bar. The mass flow rates of the HEM are inaccurate when compared to the experimental results with a relative difference of approximately 42%. This outcome was expected because the theoretical background of the model assumes that there would be choking at saturation pressure. The modification of the HRM approach was performed with the use of a genetic algorithm (GA) in order to adapt the model's constants, originally defined for water, to R410A. The HRM approach from literature using constants for water yielded average differences of 17 and 26% using two different relaxation time correlations. The modified HRM approach produced an average relative difference of around 5% for optimised relaxation time correlation constants. The study proved the feasibility of the adaptation of the HRM approach to various working fluids, both synthetic and natural.

Keywords: Refrigeration, Expansion valve, Two-phase flow, CFD model, Relaxation model, Genetic algorithm

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1. Introduction

The basic function of an electronic expansion valve (EEV) in the refrigeration cycle is to maintain the pressure difference between the high and low-pressure sections of the cycle. Regulation of the refrigerant mass flow rate (MFR) is another essential function of the EEV as it allows the regulation of the cooling load. The MFR is usually regulated by the insertion of a needle into an orifice, and used as a as a variable expansion device which is shown in Fig. 1 (a). The deeper the needle is inserted, the lower the MFR produced. The needle inside the orifice creates a channel with a varying cross-section (CS) in a similar manner to a converging-diverging nozzle. Another way to regulate the flow is to pulsate the flow utilising a pulse width modulated valve, as shown in Fig. 1 (b). In this case, the MFR depends on how long it takes a plunger to close the EEV during one time period.

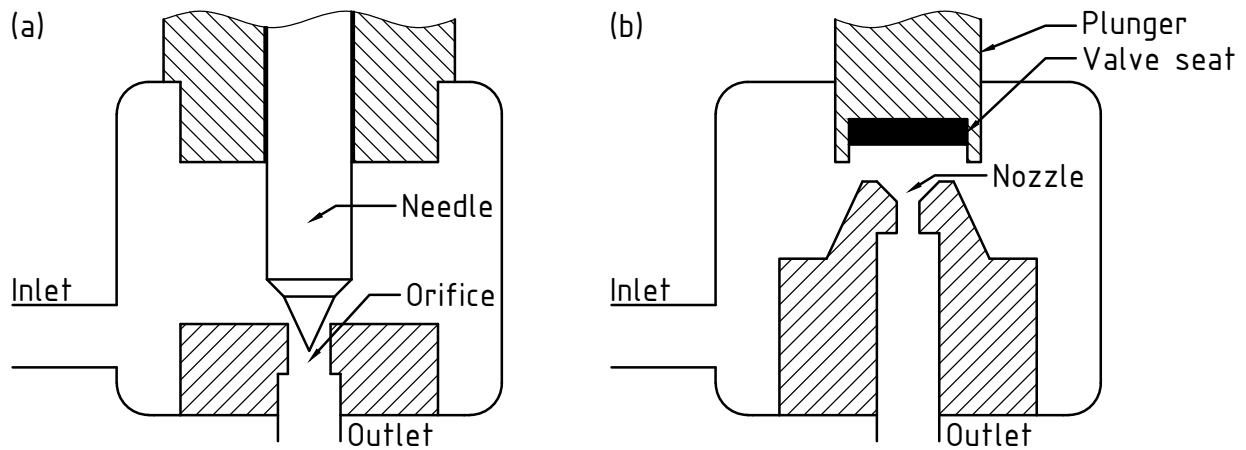


Figure 1: 1. (a) The EEV with the flow restricting needle and (b) the EEV with a periodically clogging plunger.

Fig. 1 shows the geometry of two EEVs considered converging and converging-diverging ducts which are usually found in EEVs. Flows inside the EEV, determined as compressible, single-phase fluids, are described thoroughly by the theory of gas dynamics, e.g. Zucker and Biblarz (2002). This also applies to the critical flow. The critical flow, or the choked flow, occurs when there is no further increase of the MFR with further reduction of the back-pressure. This is due to pressure disturbances propagating upstream with sonic velocity. If the velocity of the flow reaches the sonic velocity, the pressure disturbances cannot travel any further upstream (Elias and Lellouche, 1994; Moody, 1975). The only place where the single-phase fluid sonic velocity may occur in the converging and converging-diverging nozzle is at the minimum cross-section of the nozzle called the *throat*. If the pressure in the throat reaches the value providing the sonic velocity, any further reduction of the back-pressure will not affect the parameters within the throat and, consequently, the MFR. The aforementioned pressure which provides the sonic velocity is called the *critical pressure* and it should not be mistaken with the pressure corresponding to the critical point of the given fluid. For compressible single-phase flow, the critical pressure can easily be determined as a function of the stagnation pressure and the isentropic exponent.

27 There is no general equation describing the critical pressure, which is applicable to a wide
28 range of conditions and fluids for a two-phase flow of one component. This fact makes the cal-
29 culation of MFR for two-phase flow particularly difficult as the critical MFR results strictly from
30 the critical pressure (Kolev, 2015). Moreover, for **heterogeneous** two-phase flow, the sonic ve-
31 locity is no longer a thermodynamic property since it is dependent on the regime of the flow.
32 This phenomenon has been shown in the experimental investigation made by Henry et al. (1971).
33 Depending on the flow regime, e.g., slug flow, bubbly flow, separated flow, etc., the interfacial mo-
34 mentum transfer differs making the calculation of the sonic velocity for the mixture problematic.
35 Other factors affecting two-phase flow are the mechanical and thermodynamic non-equilibria. A
36 finite rate of momentum transfer between phases results in the mechanical non-equilibrium man-
37 ifesting itself into a velocity difference between the phases. The thermodynamic non-equilibrium
38 is a finite rate of heat and mass transfer between phases (Bilicki and Kestin, 1990), resulting in
39 different temperatures for these phases. In other words, the phase change requires a finite time
40 to occur and this time is called the *relaxation time*. The relaxation time is important during flow
41 simulations through short channel paths such as orifices and nozzles. A fluid particle may transit
42 a short channel path in a shorter time than the relaxation time. This results in the formation of
43 a superheated (metastable) liquid at lower pressure than in those at thermodynamic equilibrium
44 (Lahey and Moody, 1993) as the evaporation is delayed by the relaxation time, leading to a higher
45 MFR than those predicted when assuming thermodynamic equilibrium. Sallet (1991) reported that
46 the two-phase flow through a short nozzle or orifice, i.e., the flow affected by thermodynamic non-
47 equilibrium effects, has an MFR which is two or three times higher than the flow through a long
48 pipe with the same diameter as the short nozzle. This is because the pipe is a channel providing a
49 residence time long enough to establish thermodynamic equilibrium. One of the models proposed
50 by Sallet addressed two-phase water discharge from a vessel through a valve nozzle. For a vessel
51 pressure equal to 689.5 kPa and a temperature range from 90 to 160 °C, MFRs resulting from this
52 model were two to four times higher than MFRs resulting from the calculations assuming thermo-
53 dynamic equilibrium. Tong and Tang (1997) reported a clear separation between flows through
54 long channels and short channels. In long channels, thermodynamic equilibrium may be assumed,
55 and in short channels, thermodynamic non-equilibrium effects must be considered.

56 The Homogeneous Equilibrium Model (HEM), and Homogeneous Relaxation Model (HRM)
57 approaches find their applications in modelling the expansion process where a phase change oc-
58 curs. This expansion process can be a leakage of flashing coolant from a ruptured pipe in the
59 nuclear industry (Lahey and Moody, 1993), the discharge of compressed liquefied gases (Sallet,
60 1991), refrigerant expansion through ejectors (Haida et al., 2018), capillary tubes (Ingle et al.,
61 2015), or EEVs. One of the main disadvantages of HEM is the presence of strong discontinuities
62 of the sonic velocity at the saturation line. There is a significant difference between the sonic
63 velocity for the liquid and the sonic velocity for the two-phase region, even for the vapour mass
64 fraction approaching infinitely close to 0. There is an analogous difference between the sonic ve-
65 locity for the vapour and the two-phase region, although it is not as severe as the aforementioned
66 difference concerning the liquid saturation line. This discontinuity is in contradiction with the ex-
67 perimental data, according to Städtke (2006). Furthermore, Städtke presents graphs showing the
68 sonic velocity differences for a two-phase mixture of water and steam over pressure ranges from 0
69 to 50 bar. This is illustrated in Fig. 2, where the vapour mass fraction is denoted by the x symbol.

70 In Fig. 2 (a) the difference between the sonic velocity for the liquid and for the two-phase region
 71 is presented. It can be seen, that the difference is enormous. Even at 50 bar, where the difference is
 72 the lowest, it still exceeds 1,000 m/s. The difference concerning the vapour is shown in Fig. 2 (b).
 73 It can be observed that for the liquid, sonic velocity difference decreases with increasing pressure,
 while for the vapour, the difference is seemingly constant over the whole pressure range.

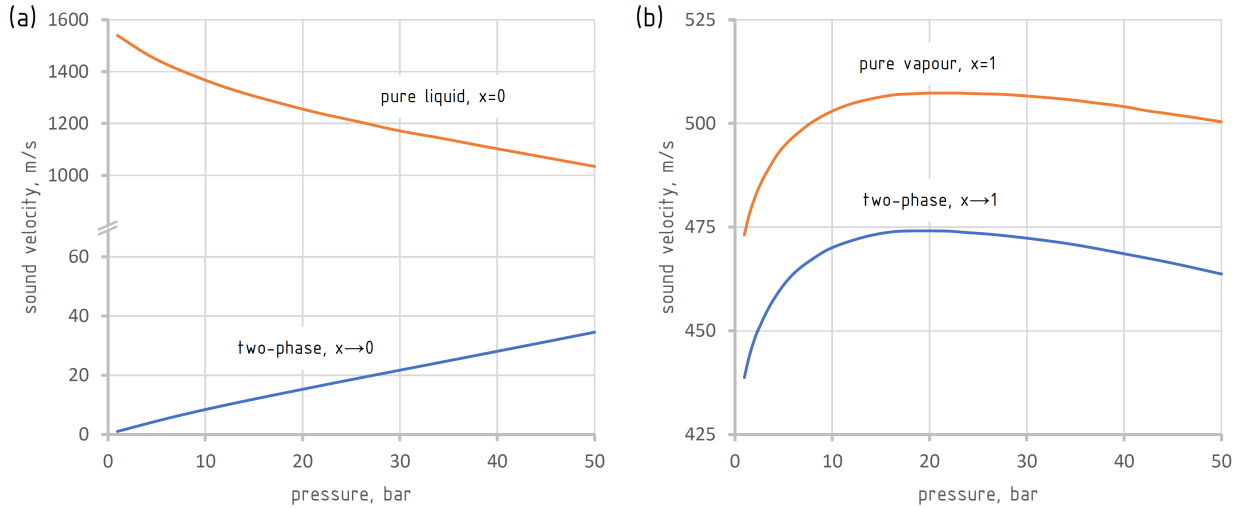


Figure 2: 2. The discontinuities of the HEM sonic velocity for (a) the liquid and (b) vapour saturation lines for H₂O (Städtke, 2006).

74 A significant discontinuity at the liquid saturation line is particularly unfortunate from the
 75 perspective of this study. An expansion line, resulting from the expansion process in the EEV,
 76 crosses the liquid saturation line. The liquid sonic velocity is so high that it is highly unlikely
 77 that the refrigerant in a liquid state will reach it while flowing through the EEV. Consequently, the
 78 liquid refrigerant may reach a higher velocity than the two-phase sonic velocity at the crossing of
 79 the expansion and the saturation lines. In this case, when the expanding refrigerant reaches the
 80 saturation line, the subsonic flow rapidly becomes supersonic, instantly choking the flow. This
 81 result from the HEM application is also reported by Städtke (2006). That author confirmed that
 82 the MFR in this case may be calculated by using a simple Bernoulli equation, Eq. (1).
 83

$$\dot{m} = C_f A_{th} \sqrt{2\rho(T_o) \cdot [p_o - p_s(T_o)]} \quad (1)$$

84 where A_{th} is the cross-sectional area of the throat, C_f is the discharge coefficient for the in-
 85 compressible liquid, and \dot{m} is the mass flow rate. The subscripts o and s denote stagnation and
 86 saturation parameters, respectively.

87 Downar-Zapolski et al. (1996) presented a graph comparing the sonic velocities between HEM
 88 and HRM with respect to the void fraction for flashing water. This graph complements Städtke's
 89 graph in Fig. 2 and shows the advantage of HRM over HEM; the lack of sonic velocity discontinu-
 90 ities between single-phase and two-phase regions. As a result, the premature choking at the liquid
 91 saturation line will not appear, allowing for deeper expansion into the two-phase region. Hence,
 92 the MFR values calculated using HRM will be higher than those calculated using HEM.

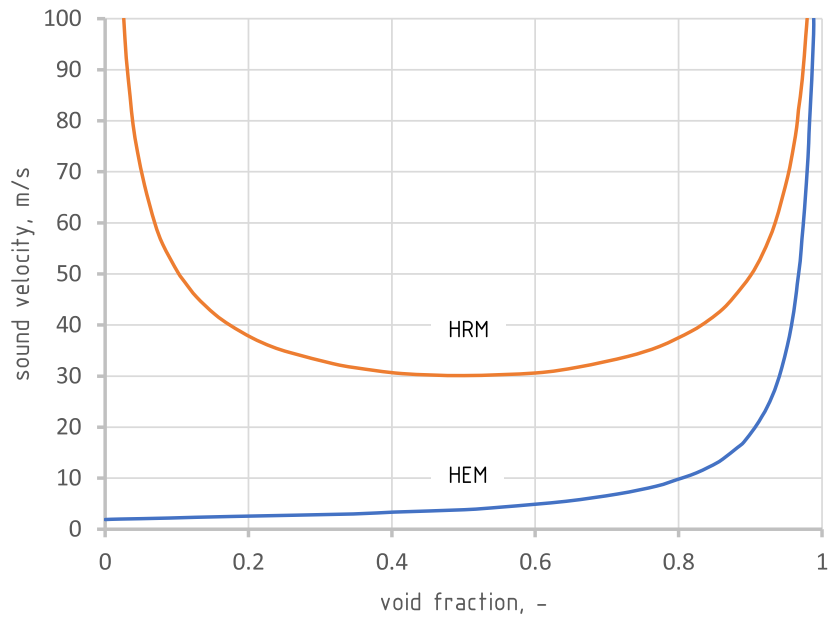


Figure 3: HRM and HEM sonic velocities for H₂O (Downar-Zapolski et al., 1996).

93 The work by Palacz et al. (2015) considered CO₂ flow through an ejector and discussed the
 94 accuracy of the HEM approach. Although it is a very specific application, this highlights the
 95 overall trend of the accuracy of HEM. The accuracy depends greatly on the operating conditions.
 96 The area close to the critical point had a very high accuracy, i.e., the MFR relative difference was
 97 approximately equal to 5%. However, a decrease in the temperature or the pressure negatively
 98 impacted the accuracy. The most reduced accuracy was found near the saturation line, where
 99 the relative differences reached up to 60%. In the work of Palacz et al. (2017a), the accuracy of
 100 HEM and HRM was given, again, for the CO₂ flow through an ejector. The HRM in the region
 101 close to the critical point provided the worst accuracy when compared to HEM and for some
 102 cases a relative difference that was twice as large as that from HEM. However, HRM provided
 103 improved accuracy in the regions where HEM had high relative differences. Unfortunately, the
 104 improvement was only 3-5 percentage points. Haida et al. (2018) considered the CFD simulation
 105 of CO₂ through an ejector and modified HRM empirical coefficients using optimisation methods to
 106 lower the discrepancy between computational and experimental data. There was an improvement
 107 of 4-19 percentage points from the HEM results. These points indicate that the empirical nature
 108 of HRM coefficients has a great impact on the MFR discrepancy and thus presents a chance for
 109 improvement.

110 The lack of any general theory behind two-phase flow means that there are numerous mod-
 111 els predicting MFR. Geng et al. (2019) modelled the two-phase expansion of a R134A refriger-
 112 erant in an ejector using a CFD approach. The metastability of the phase change was captured
 113 by adopting a finite rate phase change model developed by Yazdani et al. (2012). The resulting
 114 MFR was compared with the HEM and Abuaf and Henry-Fauske models. HEM yielded a 30%
 115 lower MFR, whilst Abuaf and Henry-Fauske models yielded a 20% higher MFR than Geng et al.
 116 (2019). Pourmahmoud et al. (2011) modelled the R410A and R22 flow through an EEV using

117 CFD by combining the HEM with the frozen flow model, with a coefficient capturing the effects
118 of metastability. The resulting MFRs were close to the experimental results from the literature pre-
119 sented by Pourmahmoud et al. (2011). However, the ideal gas equation, not suited for two-phase
120 flow, was used as an equation of state (EoS) without a comment. Grønheden (2015) investigated
121 the R410A flow through the same EEV and for the same experimental data as in this manuscript,
122 implementing HRM into the OpenFOAM software. Two correlations for the relaxation time con-
123 taining empirical constants for water yielded relative differences of 30% and 10% for MFR, with
124 respect to the experimental data. Attou and Seynhaeve (1999a,b) modelled the thermodynamic
125 non-equilibrium two-phase flow by improving the 1-D Delayed Equilibrium Model (DEM). The
126 metastability was taken into account by introducing the vaporisation index which was a mass frac-
127 tion of the metastable liquid in a two-phase mixture. The DEM improvement considered a closing
128 equation for vaporisation index modification, so the model has a good prediction of MFR for inlet
129 conditions close to the saturated liquid line. The model was used to simulate water-steam flow
130 through a pipe with abrupt enlargement.

131 For a sub-cooled liquid at the inlet, DEM and HEM provided MFRs with average relative
132 errors from the experimental results equal to 2.5% and approximately 17%, respectively. For
133 the two-phase region near the liquid saturation line with vapour mass fraction up to 6%, DEM
134 and HEM provided MFRs with average relative errors from experimental results equal to 4% and
135 approximately 28%, respectively. Saleh and Aly (2016) developed an artificial neural network
136 (ANN) to calculate the MFR for R22, R407C and R410A flowing through an EEV. The agreement
137 between calculated MFRs and the experimental MFRs were 0.7%, 1.1% and 0.006% for R22,
138 R407C and R410A, respectively. A general model considering all three refrigerants provided
139 good agreement of approximately 2.5%. Cao et al. (2016) presented an ANN predicting a MFR
140 for R410A, R407C and R22 flowing through an EEV. The ANN with a Tan-Sigmoid transfer
141 function provided an average deviation of -0.4%, 0.1% and 0.1%, respectively compared to their
142 in-house experiment, literature data and manufacturers' data. Analogously, the ANN with an x^3
143 transfer function provided an average deviation of -0.2%, 0.07% and -1.1%, respectively. By
144 experiment, Chen et al. (2019) examined the MFR of a R1233ZD refrigerant flowing through
145 an EEV by creating an ANN and power-law correlation model. The ANN and the power-law
146 correlation model provided results with a -0.2% and 0.8% average deviation, respectively. In
147 another study, Chen et al. (2017) created a power-law and polynomial correlation returning an
148 MFR of the R245FA flow through an EEV. The average deviations were 0.58% and 0.77% for
149 the polynomial correlation and power-law, respectively. In the next study, Chen et al. (2018)
150 expanded the R245FA flow investigation by using an additional three EEVs with larger orifice
151 diameters, and the resulting average deviations were 0.67% and 0.85% for the power-law and
152 polynomial correlation, respectively. Zhifang et al. (2008) developed a mass flow correlation for
153 R134A flow through an EEV characterised by a maximum error of 6.8%. Li (2013) investigated
154 experimental data from the literature for R22, R407C and R410 flow through an EEV. Based on
155 the experimental data, a polynomial correlation and an empirical correlation resulting from the
156 Buckingham π -theorem were developed to predict MFR. For the R410A the relative error ranges
157 for the polynomial correlation and the empirical correlation were $\langle -5\%, 5\% \rangle$ and $\langle -15\%, 15\% \rangle$,
158 respectively. In the literature, there is a significant amount of work which addresses empirical
159 correlations for MFR for numerous refrigerants flowing through an EEV. Empirical correlations

160 concerning R410A from Shanwei et al. (2005), Park et al. (2007) and Chen et al. (2009) provided
161 the relative deviations in the following ranges: $\langle -10.6\%, 9.9\% \rangle$, $\langle -15\%, 15\% \rangle$ and $\langle -7\%, 10\% \rangle$,
162 respectively.

163 The ANN, power-law correlation and polynomial correlation models, while being practical,
164 ignore the physics of the process and rely only on the empirical data, fitting the coefficients to
165 approximate MFR ranges with the parameters limited by the measurement scope and working fluid
166 used. The CFD approach requires a longer computational time than the above-mentioned empirical
167 correlations, providing not only the predicted MFR itself but also the physical background in the
168 form of field results with many parameters. Such results are interesting from a scientific point of
169 view since they broaden the knowledge of two-phase phenomena, and from a practical point of
170 view, since they can suggest new solutions in, e.g., the design or improvement of the operation
171 effectiveness of a particular device. However, there is a scarcity of research considering CFD
172 modelling of two-phase flow through EEVs. In this work, not only is the CFD model of two-phase
173 flow through an EEV presented, but a procedure for adapting this method to many media is also
174 presented.

175 The main objective of this work is to propose a CFD model of R410A refrigerant flow through
176 the AKV 10-2 model EEV. The HEM and HRM approaches are used to capture the generation
177 of the vapour during the phase change. The CFD model is used to predict the MFR of R410A
178 for a valve nozzle with an inlet pressure of approximately 20 bar for every operation point; the
179 outlet pressure is varied from 6.8 to 11.5 bar, and the sub-cooling range is 3.8 to 7.7 K according
180 to experimental tests carried out at the Danfoss laboratory. The valve nozzle was fully opened
181 for all operating conditions, since it allows for the most accurate acquisition of experimental data.
182 The CFD model will provide the distribution of thermodynamic parameters throughout the EEV
183 geometry that allow for a deeper understanding of metastability phenomena occurring inside the
184 valve. The 2-D or 3-D distribution of thermodynamic parameters results in global parameters, e.g.,
185 the pressure drop and MFR which can be used to assess the quality of the design of an expansion
186 device.

187 The distribution of thermodynamic parameters allows for the study of geometry effects on
188 valve performance that would not be revealed by other modelling approaches, e.g., flow separa-
189 tion, formulation of recirculation zones and near wall flow behaviour. Moreover, an analysis of
190 such distributions allows for the calculation of the distribution of the entropy generation that can
191 directly localise regions where the potential for the design improvement exists. A CFD model pro-
192 viding such results is a convenient tool for design purposes because it allows for the shape design
193 and optimisation of the expansion valve. Due to this fact, the HRM model was selected in the
194 current study, as it provides a shorter computational time in comparison to the mixture approach
195 proposed by Yazdani et al. (2012), as reported by Lee et al. (2016), making the HRM model more
196 convenient in the further design optimisation of an expansion device. It has to be noted, however,
197 that Yazdani's mixture approach was successfully implemented in the work of Bodys et al. (2020)
198 where a more complex flow was simulated through a novel design of a CO₂ ejector with a by-
199 pass duct of the suction flow. In addition, Yazdani's approach was implemented in the work of
200 Geng et al. (2019), mentioned earlier, concerning the R134A converging-diverging nozzle, while
201 a similar approach to Yazdani was adopted in the work of Baek et al. (2018) who used a R134A
202 ejector. The HRM empirical coefficients for water derived by Downar-Zapolski et al. (1996) were

203 replaced as a result of the optimisation procedure adapting the HRM approach to the R410A refrigerant
204 which minimised the discrepancy between the calculated results and the experimental data.
205 The optimisation procedure was based on a genetic algorithm (GA) and allowed for the reduction
206 of the MFR relative difference from 26% to 5%. This procedure would be a relatively simple way
207 to adapt the HRM approach from water to different working fluids.

208 2. EEV geometry and mesh

209 2.1. Geometry

210 The EEV being studied here has a geometry containing a clogging plunger. Because a fully
211 open valve is being studied, there is no need to capture the movement of the plunger during the
212 geometry generation, so the whole grid is modelled as if it were stationary. Danfoss provided a
213 3-D geometry file containing an assembly of components of the AKV 10-2 model EEV. The actual
214 feature of the valve flow channels used in the study was simplified to a fully axisymmetric
215 geometry in the mathematical model. In the work regarding the flow modelling through an ejector,
216 Palacz et al. (2016) reported that the motive nozzle mass flow rate for 2-D axisymmetric geometry
217 has a negligible difference to the 3-D MFRs by 0.14 percentage points. Pianthong et al. (2007)
218 presented the static pressure distribution along an ejector for 2-D and 3-D geometry, concluding
219 that the properties from 2-D geometry are satisfactorily close to the ones from the 3-D geometry.
220 One must note, that the 2-D axisymmetric simplification of an ejector geometry has the most significant
221 impact on the inlet channel to the suction nozzle. The final version of geometry, presented
222 in Fig. 4, was expanded in an axial direction, to maintain the value of inlet cross-section area of the
223 original assembly. The length of the additional inlet channel was chosen to exceed ten hydraulic
224 diameters so a well-developed flow profile could be acquired. In addition, the outlet section with
225 the biggest diameter was omitted to delete the recirculation area where the vortices would form.
226 Due to this, the stability of the calculations increased. Grønheden (2015) verified that the assumption
227 of neglecting the outlet section tends to have an insignificant impact on the overall results.

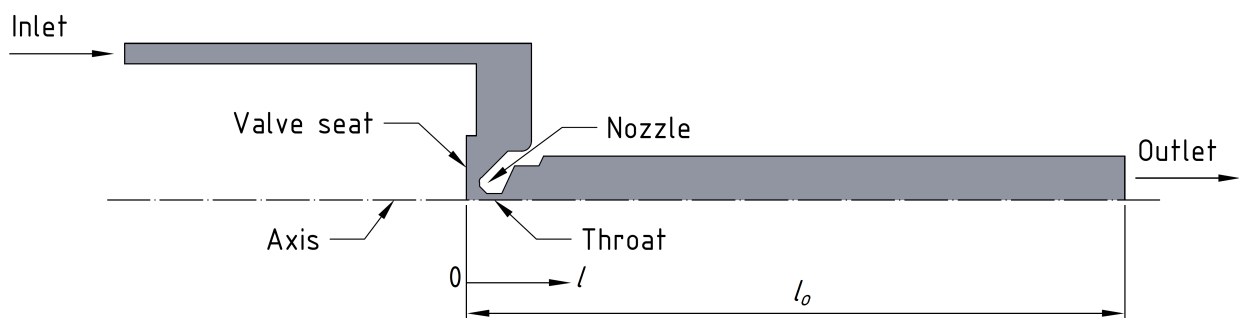


Figure 4: The final version of 2-D valve geometry.

228

229 2.2. Mesh

230 Six meshes of quadrilateral cells were generated with numbers in the range from 12,000 to
231 400,000. The exact number of cells can be found in Table 4, which contains the results of the mesh
232 independence study for the HEM calculations described in Section 4.2. Three of the characteristic
233 grids in a few selected EEV areas can be seen in Fig. 5. As the MFR prediction is the main result
234 of the model, the throat area had the most refined mesh with the aspect ratio close to 1. For even
235 more precise results considering irreversible phenomena, areas where the flow separation occurs
236 should be as refined as the throat area. However, this was not the aim of the current study.

237 3. Mathematical model

238 3.1. The HEM approach

239 The main assumptions of the model are the mechanical and thermodynamic equilibria, which
240 imply that the phases share the same temperature and velocity. Furthermore, the equality of pres-
241 sure between the phases is assumed. In other words, HEM assumes an infinite rate of heat, mass
242 and momentum transfer between phases.

243 The governing equations solved in this model (Anderson, 1995) are the mass, momentum and
244 energy conservation equations defined in Eqs (2)-(4). Steady state conditions were considered,
245 hence the lack of all-time derivatives. Eq. (2) is defined:

$$\nabla \cdot (\overline{\rho \mathbf{u}}) = 0 \quad (2)$$

246 where ρ is the density and \mathbf{u} is the velocity vector. The overline ($\overline{\quad}$) and the tilde ($\widetilde{\quad}$) above
247 the symbols denote the Reynolds-averaged and Favre-averaged quantities, respectively. Eq. (3) is
248 defined:

$$\nabla \cdot (\overline{\rho \mathbf{u} \mathbf{u}}) = -\nabla \overline{p} + \nabla \cdot (\widetilde{\boldsymbol{\tau}} + \boldsymbol{\tau}_{turb}) \quad (3)$$

249 where p is the pressure, $\boldsymbol{\tau}$ is the stress tensor and $\boldsymbol{\tau}_{turb}$ is the turbulent stress tensor. Eq. (4) is
250 defined:

$$\nabla \cdot (\overline{\rho \mathbf{u} E}) = \nabla \cdot \left[\left(\frac{\lambda}{\frac{\partial h}{\partial T}} \right)_p \nabla \widetilde{h} + \widetilde{\boldsymbol{\tau}} \cdot \widetilde{\mathbf{u}} \right] \quad (4)$$

251 where E is the total specific enthalpy, λ is the thermal conductivity, h is the specific enthalpy
252 and T is the temperature.

253 The energy equation formulation originates from the work of Smolka et al. (2013). In the cur-
254 rent study, the range of operation parameters used is located mostly in the two-phase region where
255 the temperature and the pressure are strictly bound together and cannot be used as independent
256 quantities. To amend this, Smolka et al. (2013) proposed the aforementioned energy equation,
257 Eq. (4) based on a specific enthalpy instead of the temperature. Thus, after implementation of
258 this equation as the User-Defined Scalar (UDS) feature to ANSYS Fluent (ANSYS, Inc., 2011),
259 the specific enthalpy and pressure can serve as independent variables in the single and two-phase
260 regions. Those variables were used to define the fluid properties as a function described in Eq. (5).

$$\{\rho, \mu, \lambda, c_p\} = f(p, h) \quad (5)$$

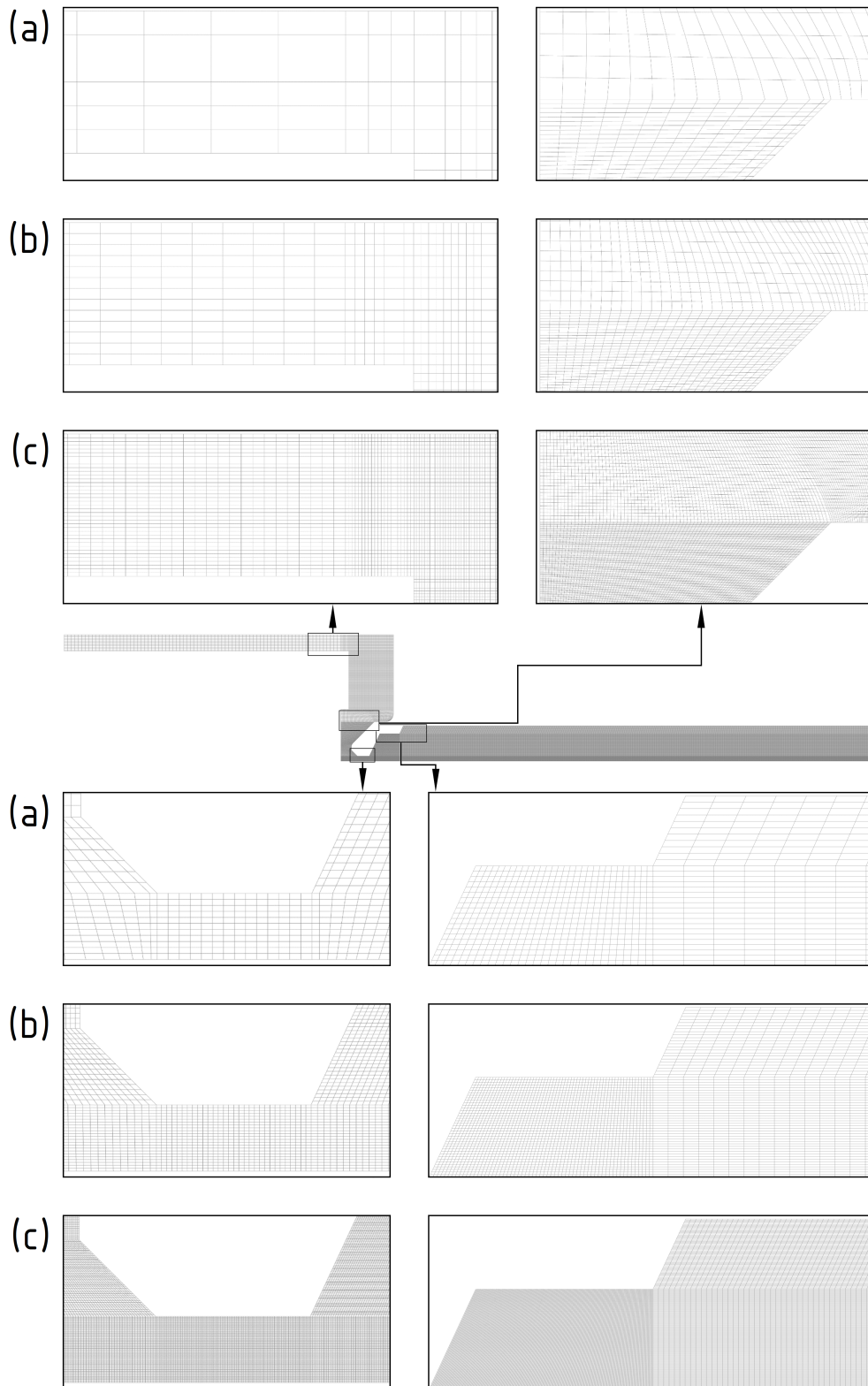


Figure 5: Meshes (a) no 1, (b) no 3 and (c) no 6 with 12, 51 and 412 thousand cells, respectively.

261 where μ is the dynamic viscosity and c_p is the specific heat capacity.

262 The properties' values were invoked as functions of the pressure and the specific enthalpy, as
 263 defined in Eq. (5), from a lookup-table for properties generated from the REFPROP 9.0 property
 264 equations, (Lemmon et al., 2010).

265 3.2. The HRM approach

266 HRM, as with HEM, assumes the equality of the phase velocities and pressures. However,
 267 HRM captures the thermodynamic non-equilibrium by introducing a concept of relaxation time,
 268 described in Section 1.

269 The governing equations of HRM comprise of all the conservation equations listed as Eqs (2)-
 270 (4). In addition, Eq. (6) which defines the vapour mass balance presented by Downar-Zapolski
 271 et al. (1996) was implemented in the same manner as Eq (4), using the User-Defined Scalar fea-
 272 ture. More details about the UDS implementation can be found in the works of Haida et al. (2018)
 273 and Palacz et al. (2017a). This equation defines the rate of vapour generation, delayed by thermo-
 274 dynamic non-equilibrium effects:

$$\frac{D\bar{x}}{Dt} = \frac{\tilde{\Gamma}}{\bar{\rho}} = -\frac{\bar{x} - \bar{x}_{eq}}{\tilde{\theta}} \quad (6)$$

275 where x is the instantaneous vapour mass fraction affected by the metastability, t is the time,
 276 Γ is the vapour generation rate, x_{eq} is the equilibrium vapour mass fraction and θ is the relaxation
 277 time. Downar-Zapolski et al. (1996) developed two correlations for θ . The first correlation for the
 278 relatively low pressures (up to 10 bar) for water was defined in Eq. (7):

$$\tilde{\theta} = \theta_{0,lp} \bar{\alpha}^{a_{lp}} \bar{\psi}^{-b_{lp}} \quad (7)$$

279 where $\theta_{0,lp}$ is the reference relaxation time equal to $6.51 \cdot 10^{-4}$ s, α is the void fraction, a_{lp} is
 280 the void fraction exponent equal to -0.257 , ψ is the non-dimensional pressure difference defined
 281 in Eq. (8) and b_{lp} is the non-dimensional pressure difference exponent equal to -2.24 . Eq. (8) is
 282 defined:

$$\bar{\psi} = \left| \frac{\bar{p}_s(T_{in}) - \bar{p}}{\bar{p}_s(T_{in})} \right| \quad (8)$$

283 where T_{in} is the inlet temperature.

284 The second correlation for the relaxation time for the water flow at relatively high pressures
 285 (above 10 bar) was used giving Eq. (9):

$$\tilde{\theta} = \theta_{0,hp} \bar{\alpha}^{a_{hp}} \bar{\phi}^{-b_{hp}} \quad (9)$$

286 where $\theta_{0,hp}$ is the reference relaxation time equal to $3.84 \cdot 10^{-7}$ s, a_{hp} is the void fraction
 287 exponent equal to -0.54 , ϕ is the non-dimensional pressure difference modified by Angielczyk
 288 et al. (2010) and b_{hp} is the non-dimensional pressure difference exponent equal to -1.76 .

$$\bar{\phi} = \left| \frac{\bar{p}_s(s_{in}) - \bar{p}}{p_c - \bar{p}_s(s_{in})} \right| \quad (10)$$

289 where s_{in} is the inlet specific entropy and p_c is the pressure corresponding to the critical point.

290 The above-mentioned modification was used to replace the inlet temperature defining the sat-
 291 uration pressure with the specific entropy. As a result, the non-dimensional pressure difference
 292 could be calculated even if parameters at the inlet were in the critical region. In the following sec-
 293 tions, the exponents from Eqs (7) and (9) along with the reference relaxation time will be described
 294 as the HRM parameters.

295 The void fraction in Eqs (7) and (9) is defined in Eq. (11):

$$\tilde{\alpha} = \frac{\tilde{x} \cdot \bar{\rho}}{\rho_v} \quad (11)$$

296 where the subscript v is the vapour saturation line property. The properties on liquid and vapour
 297 saturation lines are defined as a function of pressure, as described in Eq. (12):

$$\{\rho_v, \rho_l, \mu_v, \mu_l, \lambda_v, \lambda_l, c_{p_v}, c_{p_l}, h_v, h_l\} = f(p) \quad (12)$$

298 where the subscript l is the liquid saturation line property.

299 In the two-phase region, Eq. (5) is insufficient to capture the properties of metastable fluid. For
 300 this reason, the properties of a metastable fluid are defined in Eq. (13).

$$\{\rho, \mu, \lambda, c_p\} = f(p, h_{ml}) \quad (13)$$

301 where the subscript ml is the property in metastable conditions.

302 The specific enthalpy in metastable conditions, h_{ml} was calculated using the specific enthalpy
 303 and vapour mass fraction from governing equations (4) and (6) as defined in Eq. (14).

$$\tilde{h} = \tilde{x}\tilde{h}_v + (1 - \tilde{x})\tilde{h}_{ml} \quad (14)$$

304
 305 Eq. (15) defines the calculation of the density in metastable conditions and serves as an ex-
 306 ample since every other property under metastable conditions were calculated in an analogical
 307 manner. Eq (15) is defined:

$$\frac{1}{\bar{\rho}} = \tilde{x}\frac{1}{\rho_v} + (1 - \tilde{x})\frac{1}{\rho_{ml}(\bar{p}, \tilde{h}_{ml})} \quad (15)$$

308 The properties' values were acquired from the lookup-table for properties as described in Sec-
 309 tion 3.1.

310 3.3. Turbulence model

311 The lack of turbulence model screening in the scope of this study was compensated by the
 312 literature review which is summarised in Table 1. Table 1 comprises works where the turbulence
 313 models were investigated to simulate the ejector operation for fluids listed in the second column.
 314 The quantities used to assess global performance are listed in the third column. The last columns
 315 comprise relative errors between the calculated global quantity and experimental data. Relative
 316 errors from Croquer et al. (2016) study consider models with a high-Reynolds number. The only
 317 error presented for a model with a low-Reynolds number formulation was for $k-\omega$ SST and was

318 equal to 5.7%. Regarding Varga et al. (2017) study, case with experimental back pressure set as
 319 an outlet boundary condition was named Variant 1 and the case with calculated back pressure set
 320 as an outlet boundary condition was named Variant 2. The final recommendations in those works
 321 were proposed basing not only on accuracy of the global quantity calculation, but also on local
 322 distribution of thermodynamic parameters and advantages such as independence from wall treat-
 323 ment. The most of the authors concluded that $k-\omega$ SST was the best, except Varga et al. (2017),
 324 who concluded that Transition SST model was the best. The Realizable $k-\epsilon$ provides larger rela-
 325 tive errors than $k-\omega$ SST by, on average, 0.6 percentage points, excluding the Varga et al. (2017)
 326 outlier case for the experimental back pressure with severe underestimation of COP, which is a
 327 negligible value difference. One must note, that Mazzelli et al. (2015) considered single-phase air
 328 flow, while the rest of the presented turbulence model investigations were devoted to the ejectors
 329 with saturated vapour at the inlet of the motive nozzle, which is contrary to the condition consid-
 330 ered in current manuscript which is sub-cooled liquid at the EEV inlet. The works of Geng et al.
 331 (2019), Rusly et al. (2005) and Ingle et al. (2015) are devoted to expansion devices with similar
 332 inlet conditions as in current manuscript. The Realizable $k-\epsilon$ turbulence model was used in the
 333 work of Geng et al. (2019). The authors considered the modelling of the two-phased expansion of
 334 a refrigerant flowing through a converging-diverging nozzle inside an ejector. The same turbulence
 335 model was used by Rusly et al. (2005) in a CFD investigation of several ejector designs in a com-
 336 bined ejector cooling system. Moreover, Ingle et al. (2015) used the Realizable $k-\epsilon$ turbulence
 337 model to simulate the flow through a capillary tube. With regards to the fact that the above devices
 338 are similar to an EEV, the Realizable $k-\epsilon$ model with wall treatment set as the *Standard Wall*
 339 *Function*, was employed in the numerical part of this study. The transport equations introduced by
 340 the turbulence model are defined in the ANSYS Fluent manual (ANSYS, Inc., 2011). The model
 341 constants values were maintained at the default level.

342 3.4. Boundary conditions

343 The experimental study of R410A flow through an EEV was completed at the Danfoss labo-
 344 ratory in Denmark. Table 2 includes all the experimental data from the test rig. The data in the
 345 columns are as follows:

- 346 • the operating point (OP),
- 347 • the mass flux,
- 348 • the inlet pressure,
- 349 • the inlet temperature,
- 350 • the outlet pressure.

351 The mass flux, \dot{g} , is defined in Eq. (16):

$$\dot{g} = \frac{\dot{m}}{A_{th}} \quad (16)$$

352 For the equipment used, the accuracy was $\pm 0.15\%$ of the measured value for the Siemens Sitrans
 353 FC Mass 2100 Di 6 flowmeter, $\pm 0.05\%$ of the selected range of measured values for Wika P-
 354 10 manometers and $\pm 0,44$ K and $\pm 0,03$ K for the measurement at the EEV inlet and outlet for

Table 1: Continued summary of turbulence models literature review.

Author	Fluid	Examined global quantity		Relative error, %			
				Spalart- Allmaras	Standard $k-\epsilon$	RNG $k-\epsilon$	Realizable $k-\epsilon$
Besagni and Inzoli (2017)	H ₂ O	Entrainment ratio		1.94	12.94	0.97	2.27
Croquer et al. (2016)	R134A	Entrainment ratio		-	4.27	6.03	8.79
Varga et al. (2017)	H ₂ O	COP	Variant 1	-	33.00	26.00	42.00
	H ₂ O	COP	Variant 2	-	8.20	7.67	11.60
Mazzelli et al. (2015)	Air	Entrainment ratio		-	27.10	-	28.52

Author	Fluid	Examined global quantity		Relative error, %			
				Standard $k-\omega$	$k-\omega$ SST	RSM	Transition SST
Besagni and Inzoli (2017)	H ₂ O	Entrainment ratio		11.65	1.94	11.65	-
Croquer et al. (2016)	R134A	Entrainment ratio		-	6.78	-	-
Varga et al. (2017)	H ₂ O	COP	Variant 1	-	72.00	-	4.33
	H ₂ O	COP	Variant 2	17.93	12.27	-	4.53
Mazzelli et al. (2015)	Air	Entrainment ratio		-	27.85	27.63	-

355 Danfoss AKS21 PT1000 thermometers, respectively. The accuracy for the calibration equipment
356 was $\pm 0.12\%$ of the measured value for the flowmeter, ± 2 kPa for the manometers and ± 0.08 K
357 for the thermometers. The data from the last three columns were used to define the boundary
358 conditions. As explained in Section 3.1, the independent variables used in the calculations are the
359 specific enthalpy and the pressure. The inlet parameters from Table 2 are sufficient to acquire the
360 specific enthalpy and to define the boundary conditions with parameters appropriate to the adopted
361 governing equations. Hence, the inlet boundary condition was set to the pressure-inlet and defined
362 by the aforementioned inlet specific enthalpy and inlet pressure. The outlet boundary condition
363 was set as the pressure-outlet and defined by the outlet pressure measurement. The mass flux
364 measurements were used to validate the numerical model.

365 The general location of the eight OPs on the pressure-enthalpy graph are given in Fig. 6 (a).
366 The red marking above the rectangle is the location of all the inlet conditions. The inlet conditions
367 are fairly similar for every OP. The parameter that differs the most between the OPs is the outlet
368 pressure, i.e. the parameters at which the expansion process ends. The bold, green rectangle
369 indicates the expected area where the expansion process ends for all the OPs. The exact location
370 of each of the eight OPs can be seen in the scaled-up pressure-enthalpy graph given in Fig. 6 (b).
371 It can be seen that OPs that are seemingly similar in terms of pressure range, e.g., OP6 and OP7,

Table 2: Experimental data provided by Danfoss.

OP	\dot{g} , $\text{kg s}^{-1}\text{m}^{-2}$	p_{in} , Pa	T_{in} , K	p_{out} , Pa
1	30,956	1,965,000	300.9	1,151,000
2	32,488	1,966,000	300.9	1,086,000
3	34,330	1,963,000	301.2	936,000
4	36,272	1,965,000	301.2	807,000
5	38,013	1,965,000	301.5	682,000
6	34,807	1,963,000	298.9	936,000
7	34,673	1,963,000	297.1	935,000
8	31,567	1,967,000	297.0	1,142,000

are actually different due to the inlet specific enthalpy.

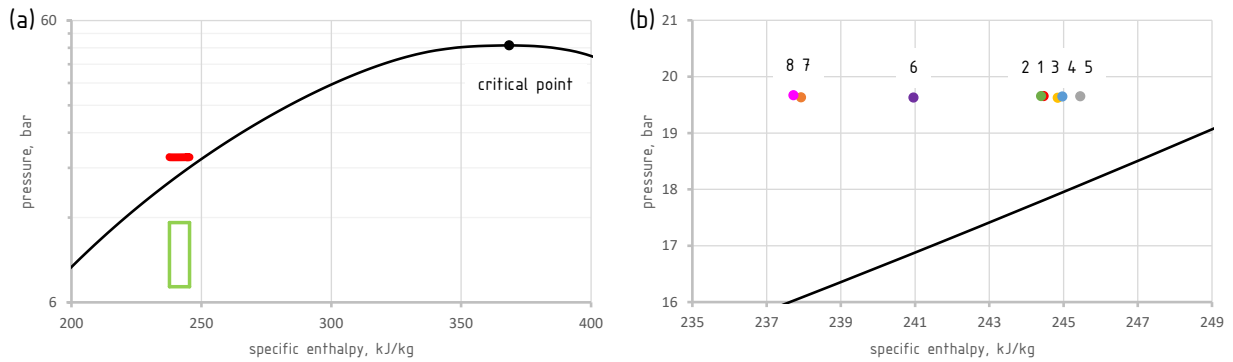


Figure 6: (a) Inlet (red marking) and outlet (green frame) boundary conditions and (b) a scaled-up view showing the inlet boundary conditions on the pressure-enthalpy diagram.

372

373 3.5. Material properties

374 The geometry only comprises of the R410A refrigerant. The refrigerant was modelled as a real
 375 fluid with its properties lookup-table generated based on the REFPROP property equations. The
 376 intervals between the lookup-table points were 5.34 kPa and 0.9 kJ/kg for the pressure and the spe-
 377 cific enthalpy, respectively. The properties corresponding to the pressure and the specific enthalpy
 378 values between the points were interpolated using bilinear interpolation functions between input
 379 parameters. The size of the lookup table was defined for 500 point of each input parameter. Hence,
 380 throughout the operating regime of EEV was within the properties table at interpolation discrep-
 381 ancy within $\pm 0.1\%$ when compared to results given directly from the REFPROP database. The
 382 roughness of the wall was unknown, and for this reason, its effect on the MFR was investigated.
 383 The HRM results of the investigation are given in Table 3. The first column contains the OPs
 384 and the following four columns contain the relative differences characterising the mass fluxes for
 385 $2 \cdot 10^{-6}$ m, $5 \cdot 10^{-6}$ m, $1 \cdot 10^{-5}$ m and $2 \cdot 10^{-5}$ m roughness heights, respectively. The relative
 386 difference results from a comparison of the mass flux for a given roughness height to the mass flux
 387 for a reference height without roughness. The final row of Table 3 contains the average relative
 388 difference for a given roughness height. Noticeably, with increasing roughness height, the mass

389 flux decreases. The only notable values of the relative difference were observed at OP3 and OP4.
 390 For these cases, the relative difference for all the roughness heights was approximately 3 and 5%
 391 for OP3 and OP4, respectively. The rest of the results were less significant and the highest average
 392 relative difference was equal to 2%. Ultimately, the overall influence on the results is insignificant.
 393 In spite of this, the case with the highest impact on MFR was chosen for all the future calculations,
 i.e., the case where the highest roughness was equal to $2 \cdot 10^{-5}$ m.

Table 3: Effect of roughness height influence on MFR.

Roughness height, m	$2 \cdot 10^{-6}$	$5 \cdot 10^{-6}$	$1 \cdot 10^{-5}$	$2 \cdot 10^{-5}$
OP	$\delta_g, \%$			
1	0.531	0.355	0.047	-0.277
2	0.442	0.209	-0.075	-0.460
3	-2.201	-2.674	-2.943	-3.209
4	-4.843	-5.145	-5.376	-5.597
5	-0.096	-0.514	-0.812	-1.288
6	-0.567	-0.896	-1.190	-1.507
7	-0.733	-1.012	-1.305	-1.663
Average, %:	1.345	1.544	1.678	2.000

394

395 4. Computational procedure

396 4.1. Solver settings

397 All numerical computations were performed using the ANSYS Fluent solver (ANSYS, Inc.,
 398 2011) under steady state conditions. The solver type was set as pressure-based and the solution
 399 method was pseudo-transient. The *Under-Relaxation Factors* for pressure and momentum were
 400 set to 0.25, and the turbulent kinetic energy and turbulent dissipation rate were set to 0.75, and the
 401 density, body forces, turbulent viscosity and specific enthalpy (UDS) were all set to 1 and, finally,
 402 the instantaneous vapour quality (UDS) was 0.04. The spatial discretisation for the pressure was
 403 set to the second order, whilst the power law was used for the turbulent kinetic energy, the turbulent
 404 dissipation rate and the specific enthalpy. For all the remaining variables, a second-order upwind
 405 was chosen. Convergence criteria were assumed to be the mass flow rate imbalance between the
 406 inlet and the outlet lower than 1% and the residual of all equations below 0.0001. For the HRM
 407 calculations, some HRM parameters caused a divergence of the computational process. The most
 408 significant problem with convergence was seen with OP8. The calculations did not diverge. No
 409 matter what HRM parameters or solver settings were chosen, the mass imbalance remained at an
 410 unacceptable level. The effect of minimum values of the absolute pressure on the cell facets of
 411 the numerical grid during iterations was monitored. The minimum facet values for cases that did
 412 not converge were oscillating greatly. The values of down peaks were negative, which is a non-
 413 physical feature of absolute pressure. As a result of this there are no results for OP8 presented in
 414 Table 3.

415 **4.2. Mesh independence study**

416 Mesh independence analysis was completed using OP1 in order to choose an appropriate mesh.
 417 Mass flux and throat pressure were the main analysis criteria used. The throat pressure is a param-
 418 eter that directly influences the mass flux and must therefore be included in the mesh independence
 419 analysis. Correctly calculating the mass flux is the purpose of this study, so it was necessary to
 420 ensure that it was independent from the mesh density. In Tables 4 and 5, the results of the mesh
 421 independence analysis for HEM and HRM are presented, respectively. In the columns, the fol-
 422 lowing quantities are presented: the mesh number, the number of mesh cells, the mass flux, the
 423 mass flux relative difference, the throat pressure, the throat pressure relative difference and the
 424 computational time. The relative difference for a given j -quantity is defined in Eq. (17).

$$\delta_j = \frac{j_i - j_{i-1}}{j_{i-1}} \quad (17)$$

425 where δ_j is the relative error corresponding to the j -quantity investigated, e.g., the mass flux.
 426 The subscript i denotes the mesh number being investigated.

427 For both HEM and HRM analyses, the maximum relative difference for the mass flux is lower
 428 than 1% and for the throat pressure 0.5%. The low values of the relative differences suggest a
 429 low sensitivity of the investigated quantities to the number of cells. However, a change in the
 430 relative difference with an increasing number of mesh cells is not asymptotic. It can be observed,
 431 in an increase of the relative difference for the mass fluxes between mesh no. 3 and 4 for the
 432 HEM analysis. To reach an asymptotic region, the relative difference must always decrease along
 433 with an increase in the number of cells. This decrease should, for increasingly refined meshes,
 434 gradually become more and more insignificant. This means that the Grid Convergence Index
 435 (GCI) procedure cannot be conducted for meshes investigated in this study. The asymptotic region
 436 is likely to be obtained for meshes with a higher number of cells, which is impractical from the
 437 perspective of the scope of this work. Nonetheless, the results are highly insensitive to the number
 438 of cells. Thus, mesh no. 3, which consists of almost 51 thousand quadrilateral cells, was chosen
 439 for all the calculations as a compromise between mesh independent results, physical field results,
 and computational time.

Table 4: Mesh analysis results for HEM.

No.	N, -	\dot{g} , kg s ⁻¹ m ⁻²	$\delta_{\dot{g}}$, %	p_{th} , Pa	δ_p , %	time
1	12,232	18,068	-	1,756,891	-	2 h 27 min
2	24,992	18,108	0.218	1,757,800	0.052	2 h 37 min
3	50,687	18,134	0.143	1,757,815	0.001	3 h 03 min
4	101,774	18,193	0.328	1,759,005	0.068	3 h 53 min
5	205,221	18,216	0.128	1,756,914	-0.119	6 h 18 min
6	412,166	18,218	0.011	1,752,980	-0.224	13 h 18 min

440

441 **5. HRM modification**

442 The HRM parameters were derived by Downar-Zapolski et al. (1996) where the Moby Dick
 443 experiments were used as the basis of the derivation. Thus, the original HRM parameters are, in

Table 5: Mesh analysis results for HRM.

No.	N, -	\dot{g} , kg s ⁻¹ m ⁻²	$\delta_{\dot{g}}$, %	p_{th} , Pa	δ_p , %	time
1	12,232	34,035	-	1,261,199	-	0 h 48 min
2	24,992	34,237	0.596	1,258,036	-0.251	0 h 52 min
3	50,687	34,242	0.012	1,257,902	-0.011	1 h 03 min
4	101,774	34,570	0.958	1,260,598	0.214	1 h 24 min
5	205,221	34,776	0.596	1,266,479	0.467	2 h 46 min
6	412,166	34,973	0.568	1,268,842	0.187	7 h 03 min

444 fact, empirical parameters applicable to a two-phase water flow simulation. There has previously
 445 been an attempt, mentioned in Section 3.2, to adapt these parameters to other fluids. Angielczyk
 446 et al. (2010) not only changed the definition of the non-dimensional pressure difference but also
 447 adjusted the value of the reference relaxation time from the original value of $3.84 \cdot 10^{-7}$ s derived
 448 by Downar-Zapolski et al. (1996) to $2.14 \cdot 10^{-7}$ s. This was completed in order to lower the
 449 discrepancy between the experimental data and the results of the calculations for CO₂ flow through
 450 an ejector that employed the HRM approach. In the previously mentioned work of Haida et al.
 451 (2018), complex procedures such as the GA were employed to change the HRM parameters and
 452 find optimal ones which provide the lowest discrepancy between computational and experimental
 453 data. The HRM parameters obtained provided the motive nozzle MFR for pressures below the
 454 critical point with an average relative difference lowered by 5.8 percentage points when compared
 455 to the average relative difference provided by Angielczyk et al. (2010) HRM parameters.

456 In recent work, an approach similar to the one used by Haida et al. (2018) was adopted. The
 457 HRM parameters were optimised using the same GA. This GA was also described and successfully
 458 used in the works concerning an ejector shape optimisation reported by Palacz et al. (2016, 2017b).
 459 The GA has the following parameters: the probability of uniform crossover, mutations and creep
 460 mutations set to 50%, 2% and 4%, respectively. The elitism option was used and the number
 461 of genes was set to 9. An individual gene consisted of three chromosomes i.e. these were the
 462 arguments of an objective function, OF . These arguments were the empirical constants defining
 463 the relaxation time in Eq. (9). The OF was defined according to Eq. (18).

$$OF(\theta_0, a, b) = \frac{1}{n} \sum_{i=1}^n \left| \frac{\dot{m}_{cal, i} - \dot{m}_{exp, i}}{\dot{m}_{exp, i}} \right| \quad (18)$$

464
 465 The subscripts exp and cal denote the experimental and computational results, respectively.
 466 This is an average value of n relative differences. In the first optimisation configuration (C1),
 467 four OPs were chosen: OP1, OP3, OP5 and OP6. The population consisted of 6 individuals. In
 468 the second optimisation configuration (C2), all OPs except OP8 were chosen and the population
 469 consisted of 20 individuals.

470 To define the search range for each chromosome, an investigation into the HRM parameters
 471 was carried out. The investigation utilised Eq. (9) which is proposed for water at relatively high
 472 pressures. The main aim was to examine the influence of the reference relaxation time θ_0 and
 473 exponents a and b on the OF over broad ranges to find the general positions of the minima and

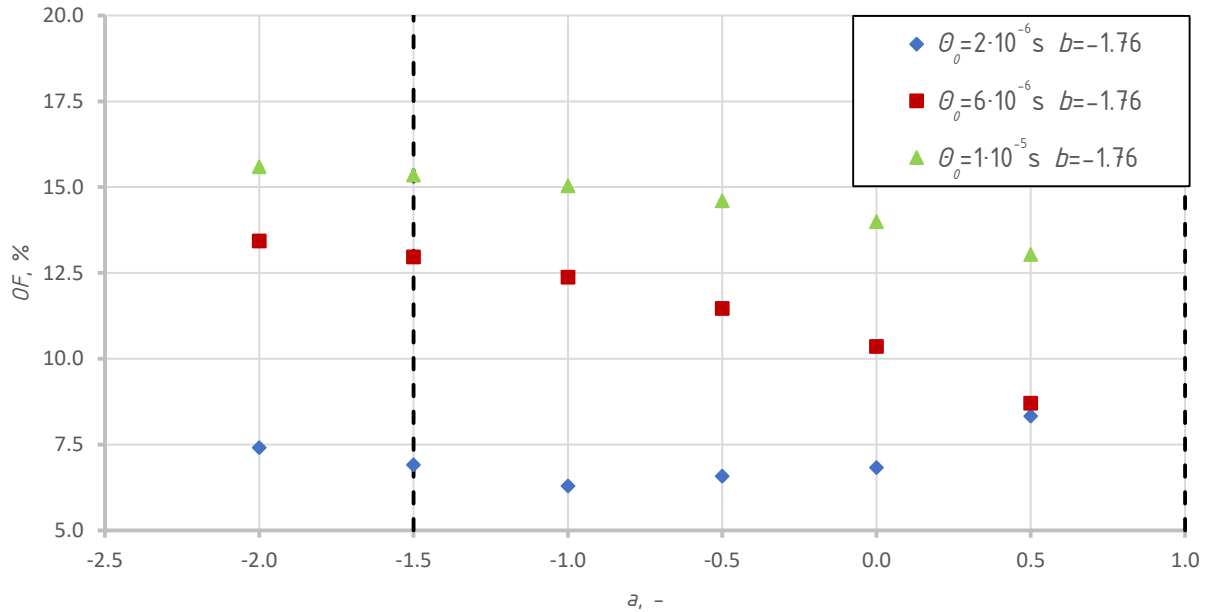


Figure 7: The influence of the exponent a on the OF value.

474 to define narrower search ranges around them. The influence of a on the OF can be seen in Fig.
 475 7, whilst the influence of b on OF is given in Fig. 8, for three values of θ_0 . When examining
 476 the influence of a , the value of b was chosen according to Downar-Zapolski et al. (1996). The
 477 exponent b was examined in a similar manner.

478 The upper limits of the broad ranges were limited by the convergence of calculations, while the
 479 lower limits resulting from decreasing values of exponents provided increasing values of OF . The
 480 dashed, vertical lines represent the defined narrow ranges of the search around the minima. The
 481 lower limits of the search ranges were set to capture the minimum associated with $\theta_0 = 2 \cdot 10^{-6}$ s.
 482 The upper boundary of the search ranges were set with the same parameters as the broad ranges.
 483 Moreover, at the upper boundary, the minimum could be closer to the central value of the reference
 484 relaxation time $\theta_0 = 6 \cdot 10^{-6}$ s, especially in the case of the b exponent. Thus, the search range for
 485 θ_0 was chosen from $2 \cdot 10^{-6}$ s to $6 \cdot 10^{-6}$ s. For the exponents, the search range for a was chosen
 486 from -1.5 to 1.0 and for b from -2.5 to -0.9.

487 **The optimised HRM parameters together with the obtained OF minima are presented in Table**
 488 6. For C1, the optimisation procedure was set to 30 generations, although the minimum OF value
 489 was already reached after the 19th generation. The minimum OF for C2 presented in the table was
 490 achieved by the 12th generation. The minimum OF for C1 and C2 are highlighted in bold font.
 491 The seven OPs were taken into account for OF_{C2} , which gives a better representation of the final
 492 result. However, OF_{C2} had an insignificantly better final result ($5.27\% < 5.28\%$) than OF_{C1} . The
 493 relative difference for the rest of the OPs and a detailed description of the results are presented in
 494 Section 6.2.

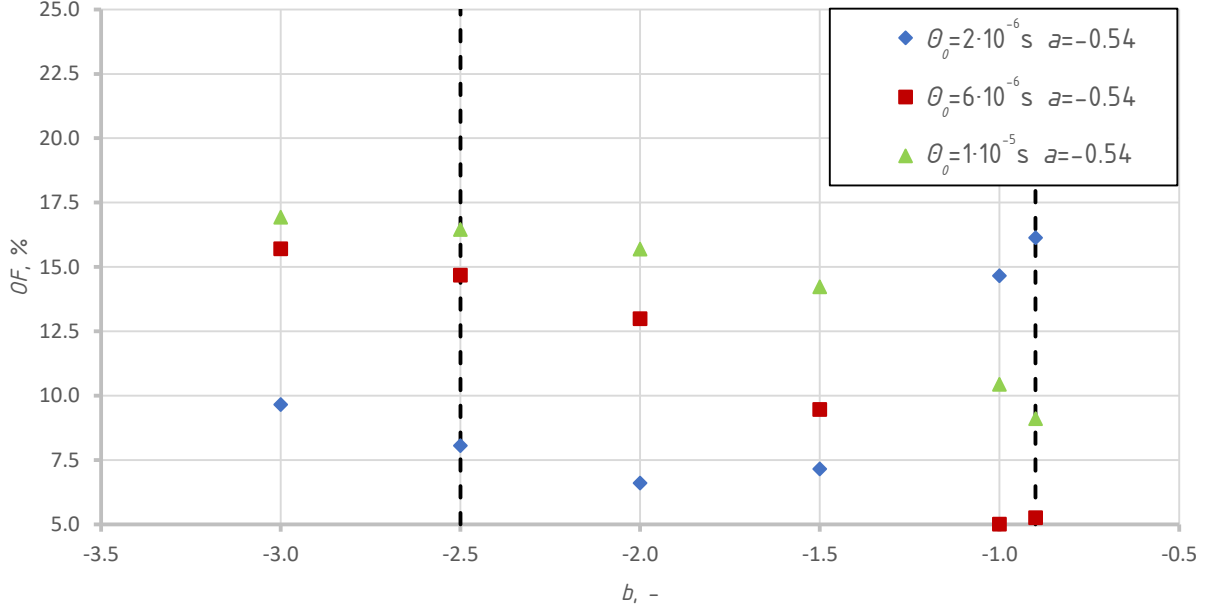


Figure 8: The influence of the exponent b on the OF value.

Table 6: The optimised HRM parameters.

	$OF_{C1}, \%$	$OF_{C2}, \%$	θ_0, s	$a, -$	$b, -$
C1:	4.92	5.28	$4.98 \cdot 10^{-6}$	-0.587	-1.100
C2:	4.87	5.27	$5.64 \cdot 10^{-6}$	-0.687	-0.968

495 6. Results and discussion

496 6.1. HEM results

497 The relative differences (denoted as δ) for the mass flow rate calculated using the HEM model
498 are presented in Table 7. The relative differences are defined in accordance with Eq. (17) and
499 for this case the subscripts i and $i - 1$ denote the calculated and experimental MFR, respectively.
500 Similarly, the subscripts are used in Eq. (18) for defining the OF . The second and third columns
501 contain the HEM results and the relative differences, respectively. The next two columns contain
502 the numerical results from HEM vs the Bernoulli equation. In the sixth column, the saturation
503 pressure is given. The last two columns contain the mass flux resulting from an isentropic expan-
504 sion, defined in Eq. (19), and the relative difference δ_{s_o} , between the Bernoulli and isentropic mass
505 fluxes. Eq (19) is defined

$$\dot{m} = C_f A_{th} \rho(p_{sat}, s_o) \sqrt{2[E - h(p_{sat}, s_o)]} \quad (19)$$

506 where $\rho(p_{sat}, s_o)$ is the density and $h(p_{sat}, s_o)$ is the specific enthalpy, which are both at the
507 throat. The root denotes the velocity resulting from the energy conservation for the adiabatic flow
508

509 with no work done. The discharge coefficient C_f was assumed as given by Chen et al. (2009) as
 510 0.94. The calculations were completed to investigate the influence of the potential density change.
 511 As can be seen, the highest relative difference is -0.13%. Hence, the influence due to the density
 512 change is negligible, as predicted.

513 The average relative difference obtained using the HEM formula was 42.25%. This result
 514 is unsatisfactory, however not unexpected. As predicted in Section 1, the flow choked on the
 515 saturation pressure resulting in a significant underestimation of the MFR. The expansion process
 516 of the still incompressible liquid, starting from operating points in the sub-cooled region, was
 517 unrestricted due to the tremendously high sonic velocity in the liquid region. This allows the
 518 liquid to achieve a velocity higher than the low sonic velocity of the two-phase region before
 519 reaching the saturation line. The saturation line is the place where a severe HEM sonic velocity
 520 discontinuity occurs. The liquid, which is still accelerating, reaches the saturation line where, due
 521 to the presence of a discontinuity, the sonic velocity drops below the flow velocity. This results
 522 in an abrupt transition from subsonic to supersonic flow and immediate choking as shown by
 523 Downar-Zapolski et al. (1996). With the assumption of the infinite rate of heat and mass transfer,
 524 the throat pressure cannot be lower than the saturation pressure which results in relatively low flow
 525 velocities and, thus, low MFRs.

526 The expansion process between the OP conditions and the saturation pressure **concerns only**
 527 the liquid. Thus the choked MFR resulting from the HEM approach should be easily calculated
 528 from the Bernoulli equation (Eq. (1)); this was mentioned in the earlier reference to Städtke. To
 529 confirm this, the results from Eq. (1) and the relative differences between the HEM calculations
 530 are presented in the fourth and fifth columns of Table 7. The average relative difference is 4.95%.
 531 For the last three points, the mass flow rates obtained, based on Eq. (1), significantly exceeded
 532 those from HEM. This is due to the fact that the Bernoulli equation provides 1-D results, while the
 533 CFD calculation provides 2-D results, presented in Fig. 9 and described in more detail in the next
 paragraph.

Table 7: HEM mass fluxes and relative differences.

OP	\dot{g}_{HEM} kg s ⁻¹ m ⁻²	δ_{HEM} %	\dot{g}_{bern} kg s ⁻¹ m ⁻²	δ_{bern} %	p_{sat} Pa	\dot{g}_{s_o} kg s ⁻¹ m ⁻²	δ_{s_o} %
1	18,134	-41.42	18,319	1.02	1,783,824	18,305	-0.08
2	18,182	-44.04	18,429	1.36	1,781,959	18,415	-0.08
3	17,820	-48.09	17,644	-0.99	1,794,105	17,632	-0.07
4	17,788	-50.96	17,568	-1.24	1,797,386	17,556	-0.07
5	17,501	-53.96	16,872	-3.59	1,810,554	16,861	-0.07
6	20,731	-40.44	22,560	8.83	1,690,588	22,536	-0.11
7	23,160	-33.21	25,745	11.16	1,611,841	25,712	-0.13
8	23,401	-25.87	26,074	11.42	1,606,663	26,040	-0.13
Average:	-	42.25	-	4.95	-	-	0.09

534 **The relative differences between the CFD and Bernoulli equation results are small enough to**
 535 **conclude that choking takes place at the saturation line. Therefore, the underestimated HEM mass**
 536 **flow rates result from the assumptions of the HEM model. The evaporation front expressed by the**
 537

538 saturation pressure isobar is presented in Fig. 9. The lower limit of the pressure field indicates
 539 the isobaric saturation pressure profiles for selected OPs. The colour maps of the pressure range
 540 are separate for each profile. This is necessary since the lowest value of the range must be the
 541 saturation pressure appropriate for each OP. The upper value of the range is the inlet pressure. The
 542 order of the OPs starts from the profiles with the shape closest to a straight line. For a low differ-
 543 ence between the inlet and the saturation pressure, the profile of the saturation pressure at the throat
 544 is close to a straight line (representing the choking plane) corresponding to the 1-D approach of the
 545 Bernoulli equation. With an increasing difference between the inlet and the saturation pressure, the
 546 saturation pressure profile loses its similarity to a straight line and tends towards a quasi-parabolic
 shape. Thus, higher pressure than the saturation pressure can be found at the choking plane.

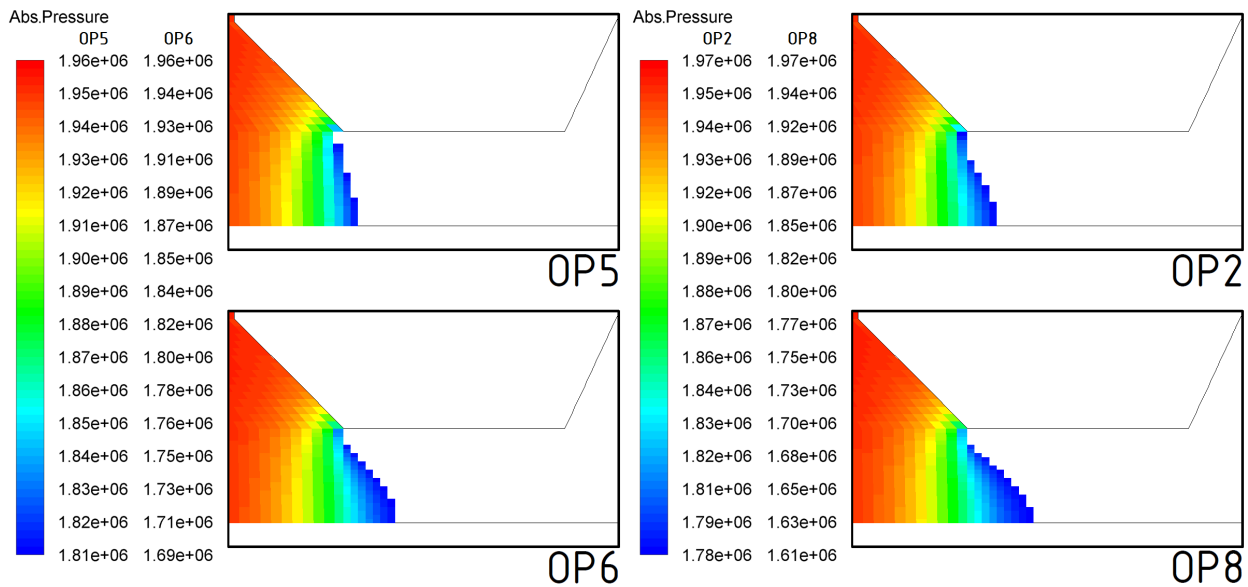


Figure 9: The lower limit of the pressure field results, indicating isobaric profiles for the saturation pressure inside the valve throat for various OPs.

547 Finally, one can conclude that the HEM model is, at the very least, inadequate for the condi-
 548 tions examined. Further description of the HEM results will be given while comparing the HEM
 549 results with the HRM results in Section 6.2.
 550

551 6.2. HRM results

552 In this section, five variants of the HRM parameters acquired from the literature and the optimi-
 553 sation procedure are addressed. Table 8 contains all of the parameter variants and their definitions:

- 554 • *Variant 1:* the Low-pressure variant which refers to the Downar-Zapolski et al. (1996) HRM
 555 parameters characterised in Eq. (7).
- 556 • *Variant 2:* the High-pressure variant which refers to the Downar-Zapolski et al. (1996) HRM
 557 parameters characterised in Eq. (9).
- 558 • *Variant 3:* custom parameter calculations (CPC) variant containing $\theta_0 = 3.84 \cdot 10^{-6}$ s.

- *Variant 4*: C1 variant which is a result of CPC parameter optimisation using only four OPs.
- *Variant 5*: C2 variant which is a result of CPC parameter optimisation using seven OPs.

Haida et al. (2018) performed a parametrisation procedure of each relaxation time constant in the R744 two-phase ejector to evaluate an influence of θ_0 , a exponent, and b exponent on the metastable flow behaviour. The authors stated that the most significant parameter that caused a delay in the flow evaporation during flashing process was θ_0 . Therefore, θ_0 defined for Variant 1 for low-pressure fluid was much higher when compared to Variant 2 for high-pressure fluid due to the different relaxation time value at the specified pressure ranges. Furthermore, an increase of θ_0 accelerated the flashed flow during expansion in the two-phase region near saturation liquid. A decrease of the a exponent described the void fraction that caused higher impact of the local void fraction on the relaxation time. According to Haida et al. (2018), an increase of a exponent caused an increase of the pressure gradient in the two-phase metastable region near the saturation liquid. The influence of the non-dimensional pressure ratio has a higher impact when the flow is expanded near the critical point (Haida et al., 2018). Furthermore, an increase of the b exponent affected the pressure gradient decrease in the two-phase region near the saturation liquid.

Table 8: HRM parameter variants.

Variant	Name	θ_0 , s	a , -	b , -
1	Low-pressure	$6.51 \cdot 10^{-4}$	-0.257	-2.240
2	High-pressure	$3.84 \cdot 10^{-7}$	-0.540	-1.760
3	CPC	$3.84 \cdot 10^{-6}$	-0.540	-1.760
4	C1	$4.98 \cdot 10^{-6}$	-0.587	-1.100
5	C2	$5.64 \cdot 10^{-6}$	-0.687	-0.968

The calculations for Variant 1 of OPs 5 and 8 did not reach a final convergence. The rest of the OPs resulted in overestimated MFRs and the average relative difference is 17.38%. The calculations for Variant 2 resulted in underestimated MFRs which are expected at low values of θ_0 . The average relative difference for OPs from 1 to 4 is 26.44%. The OPs from 5 to 8 did not achieve the assumed maximum mass imbalance, which is similar to the convergence problems described at the end of Section 3.5. A longer relaxation time should result in a higher MFR, therefore the value of $\theta_0 = 3.84 \cdot 10^{-7}$ s from Variant 2 was arbitrarily multiplied by 10 to positively affect the relative differences. Using a new value of $\theta_0 = 3.84 \cdot 10^{-6}$ s assigned as Variant 3, the results were in surprisingly good agreement with the experimental results. Only OP8, as mentioned in Section 3.5 above, did not reach the assumed maximum mass imbalance. Therefore, all further discussions will consider OPs from 1 to 7. The average relative difference for OPs from 1 to 7 was 8.18%. The case for a relatively broad range of the HRM parameters converged. This fact means that Variant 3 is suitable for optimisation and will be used in further calculations.

In Fig. 10, the relative differences are shown for the HRM calculations. Average relative differences of 8.18%, 5.28% and 5.27% were obtained for Variant 3, Variant 4 and Variant 5, respectively. As discussed in Section 1, the sub-cooled liquids expanding through nozzles into the two-phase region are influenced by thermodynamic non-equilibrium, as confirmed by satisfactory

591 agreement with experimental results. The metastability presence allows for a deeper decompression of the superheated liquid, which remains at high density. This, in turn, results in high MFRs in comparison to HEM and hence the lower values of the relative differences for the optimised HRM parameters. Although, for OP5, both optimised HRM calculations underestimated the measured mass flow rate, which resulted in a higher relative difference.

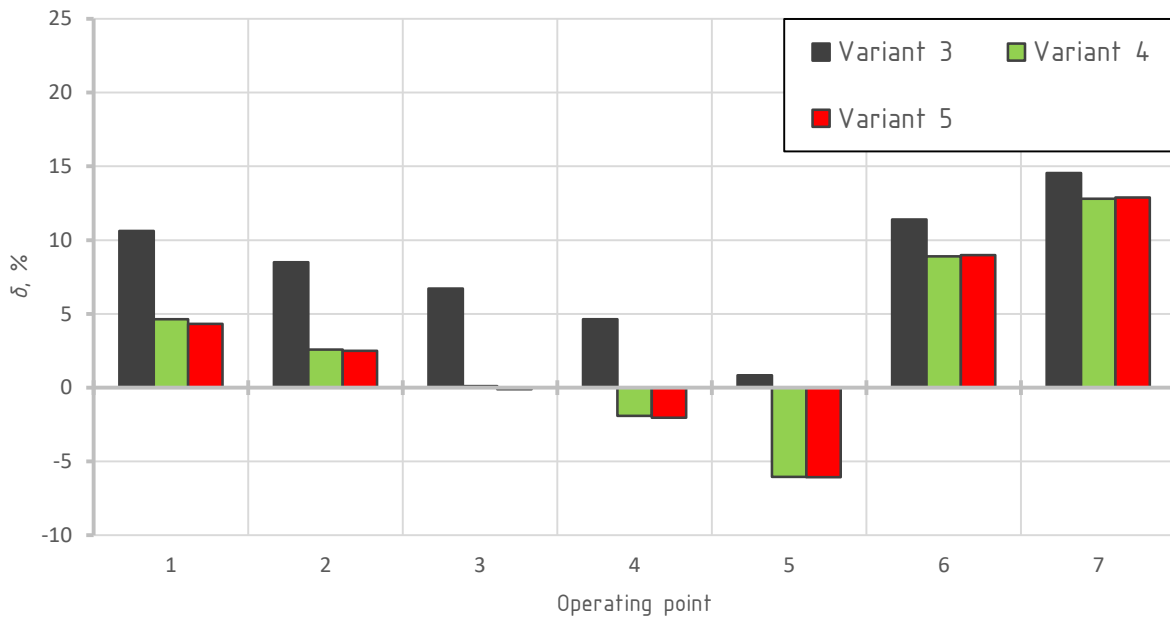


Figure 10: The relative differences between the experimental and the HRM mass flow rate for Variants 3-5.

595 The axial distribution of the pressure and velocity along the EEV for OP1 was compared between Variant 4 and 5. The average relative differences are 0.05% and 0.28% for the pressure and velocity, respectively. These values confirm that the difference between Variants 4 and 5 is negligible. Hereinafter, all the results concerning the HRM are represented by the results from Variant 5 because the lowest discrepancy is found between them and the measurement data.

601 The reference relaxation times and pressures at the inlet of the main nozzles of the expansion devices are compared for the current study and data available in the literature, see Table 9. Since HRM parameters for R410A cannot be found in the literature, the examples in Table 9 used CO₂. The general trend, although not monotonic, is that lower pressure corresponds to a higher reference relaxation time.

606 The field results of the pressure and the density for HEM and HRM are shown in Fig. 11 and Fig. 12, respectively. These results were obtained for OP1. The pressure fields for HEM show that the pressure at the throat and the constant CS channel is near the saturation pressure (1,783,824 Pa for OP1, see Table 7). This is consistent with the discussion above with regard to the HEM and Bernoulli equation results, indicating that choking takes place at the saturation line. In the HEM density field, a significant drop can be seen at the saturation pressure profile location; the location presented in Fig. 9. These low-density values characterise the isentropic expansion for

Table 9: Reference relaxation time comparison.

Source of data	p_{in} , bar	p_{in}/p_c , %	θ_0 , s
Angielczyk et al. (2010)	91.00	123	$2.00 \cdot 10^{-7}$
Haida et al. (2018)	≥ 73.77	≥ 100	$1.00 \cdot 10^{-7}$
	(59.00, 73.77)	(80, 100)	$9.00 \cdot 10^{-6}$
Current study	< 59.00	< 80	$1.50 \cdot 10^{-6}$
	19.64	27	$4.98 \cdot 10^{-6}$
	19.64	27	$5.64 \cdot 10^{-6}$

613 pressures lower than the saturation pressure because of the thermodynamic equilibrium assumption.
614 The pressure values for HRM are much lower than those for HEM. In the throat, the pressure
615 is approximately 1,300,000 Pa. Despite such a low-pressure value and the fact that the expansion
616 entered the two-phase region, the density remains at 1,046 kg/m³, which is a typical value for
617 the liquid. The HRM density field result visualises the superheated, metastable liquid presence at
618 pressures at which thermodynamic equilibrium provide much lower density values. The thermo-
619 dynamic non-equilibrium effect is observable in the throat and can also be confirmed using the real
620 fluid EoS, which in the following example were the REFPROP property functions. For OP1, the
621 inlet specific entropy $s_o = 1,151$ J/(kg · K) and the aforementioned pressure $p = 1,300,000$ Pa
622 resulted in a density of ~ 382 kg/m³, not 1,046 kg/m³, which can be seen in the HRM density field
623 results. The observable thermodynamic non-equilibrium effects, captured by the HRM approach,
624 gave higher MFRs than HEM.

625 The axial density distribution along the EEV is shown in Fig. 13 and Fig. 14. The quantity
626 defining the abscissa is a dimensionless length. It is determined by dividing the actual position
627 along the EEV, l , by the total length of the EEV, l_o . Fig. 13 shows the HEM density and REFPROP
628 density $\rho = f(p, s_o)$ where the pressure p is changing along the EEV and the parameter s_o
629 is the inlet specific entropy. HEM assumes thermodynamic equilibrium which means that all
630 the parameters are in agreement with a real fluid EoS, whether it is a pressure enthalpy chart or
631 REFPROP equations. However, the discrepancy may be observable inside the abrupt diffuser. The
632 expansion in the abrupt diffuser may no longer be treated as isentropic. In fact, this is the place
633 where the entropy rise occurs, due to the lost potential of the high inlet pressure. For the same
634 pressure, the density corresponding to s_o is higher than the density corresponding to the entropy
635 which is higher than s_o . For instance, at location $l/l_o = 0.07$, where the pressure is 1,354,210 Pa,
636 the entropy is equal to 1,154 J/(kg · K). For these parameters, the density is equal to 407.8 kg/m³
637 which is lower than $\rho = f(p = 1,354,210 \text{ Pa}, s_o = 1,151 \text{ J/(kg} \cdot \text{K)}) = 422.6 \text{ kg/m}^3$.

638 Fig. 14 depicts the thermodynamic non-equilibrium effect for HRM. The density from the EoS
639 reflects the pressure change along the EEV, while the HRM remains at a liquid density, despite
640 the pressure decrease. The highest differences between HRM and the EoS density, which are
641 approximately equal to 600 kg/m³, also indicate the location of the most significant metastability.
642 The metastability effect occurs suddenly in the middle of the nozzle and at $l/l_o = 0.065$ starts to
643 fade.

644 Fig. 15 presents the field results for the velocity for HEM and HRM. The velocity before the
645 abrupt diffuser for HEM is lower than the one for HRM, which is a result of depressurisation lim-

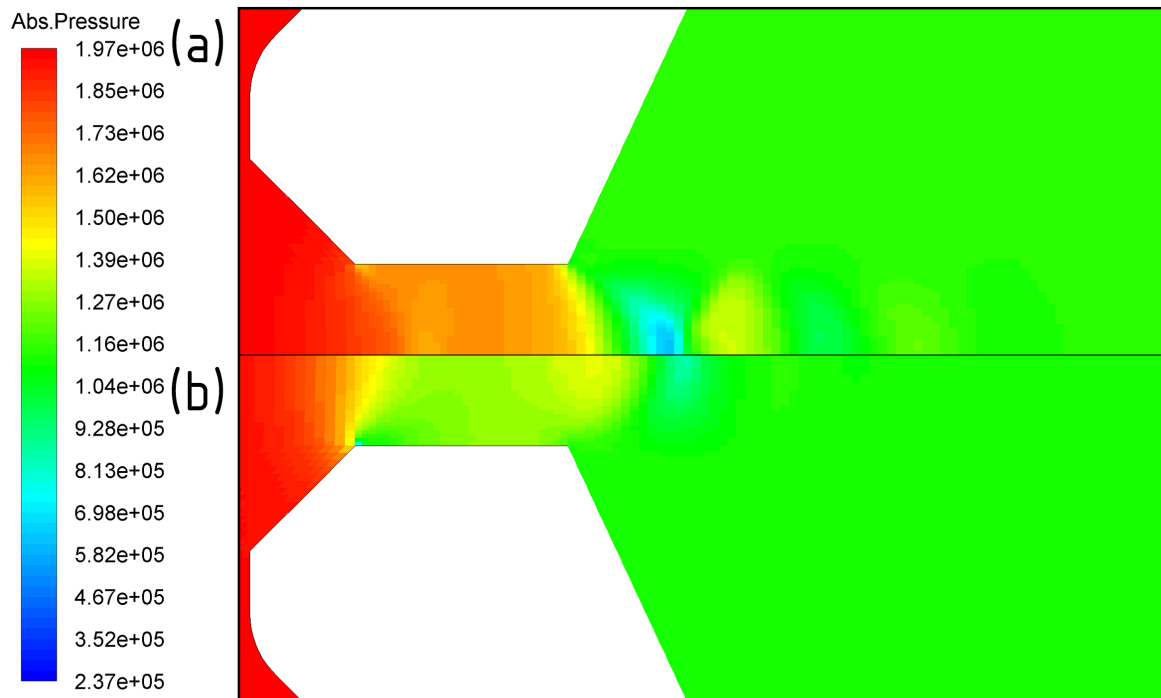


Figure 11: A comparison of the pressure in (Pa) for OP1 between (a) HEM and (b) HRM for Variant 5.

646 ited by the saturation pressure. Due to this fact, a higher pressure drop occurs in the abrupt diffuser
 647 which results in a higher HEM velocity near the shockwave by approximately 38 m/s compared to
 648 the HRM velocity. In addition, the HRM velocity increase associated with the shockwave occurs
 649 further downstream when compared to the location of the HEM velocity increase.

650 Fig. 16 presents the field results of the vapour mass fraction for HEM and HRM. For HEM,
 651 the fluid enters the two-phase region at the entrance of the constant CS channel and then, in the
 652 abrupt diffuser, the vapour mass fraction significantly increases to approximately 22.4% due to the
 653 significant pressure drop. For HRM, the constant CS channel is filled with the metastable liquid,
 654 thus the vapour mass fraction is 0%. Inside the abrupt diffuser, the vapour mass fraction increases
 655 due to the fact that the metastable liquid core is terminated by the shockwave.

656 7. Conclusions

657 Both HEM and HRM models were used in the CFD analysis of R410A refrigerant flow through
 658 an EEV. The HRM parameters were optimised to minimise the model's MFR discrepancies. The
 659 influence of the HRM parameters was investigated to define the search range for the optimisation
 660 procedure. The results of HEM and HRM calculations were compared with laboratory measure-
 661 ments. The HEM results were also compared to the analytical solution to show the agreement of
 662 the results with the model assumptions. The HRM outputs were compared with different HRM
 663 parameters to show the effect of the optimisation. The field results and graphs with an axial

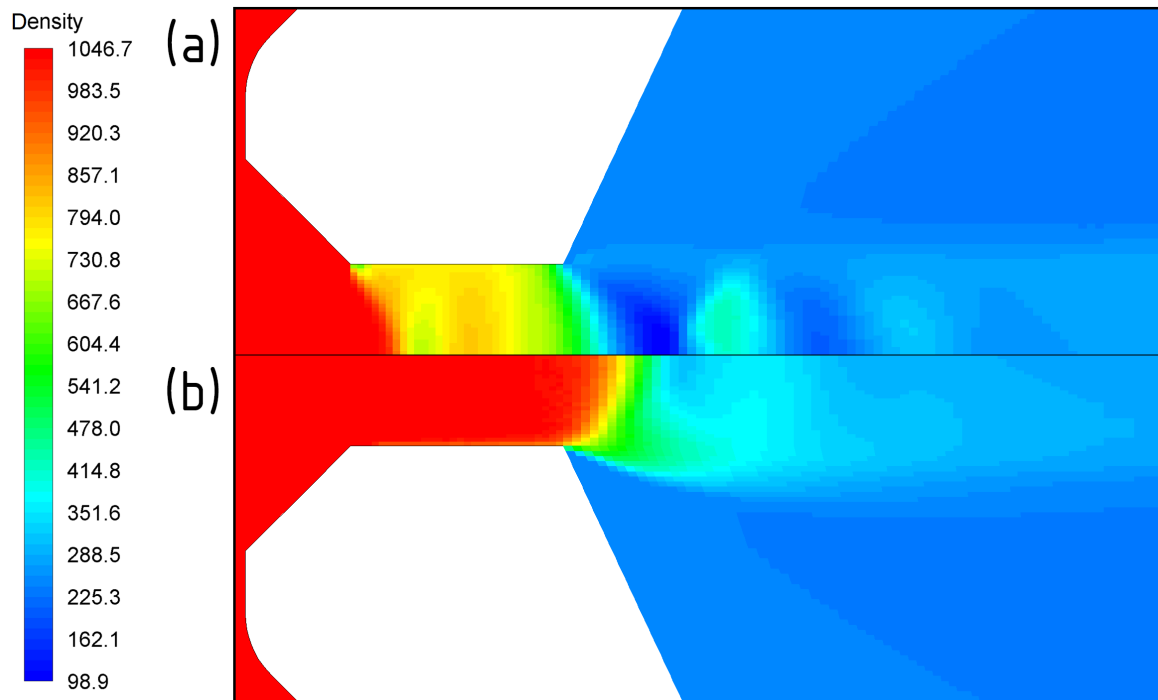


Figure 12: A comparison of the density in (kg/m^3) for OP1 between (a) HEM and (b) HRM for Variant 5.

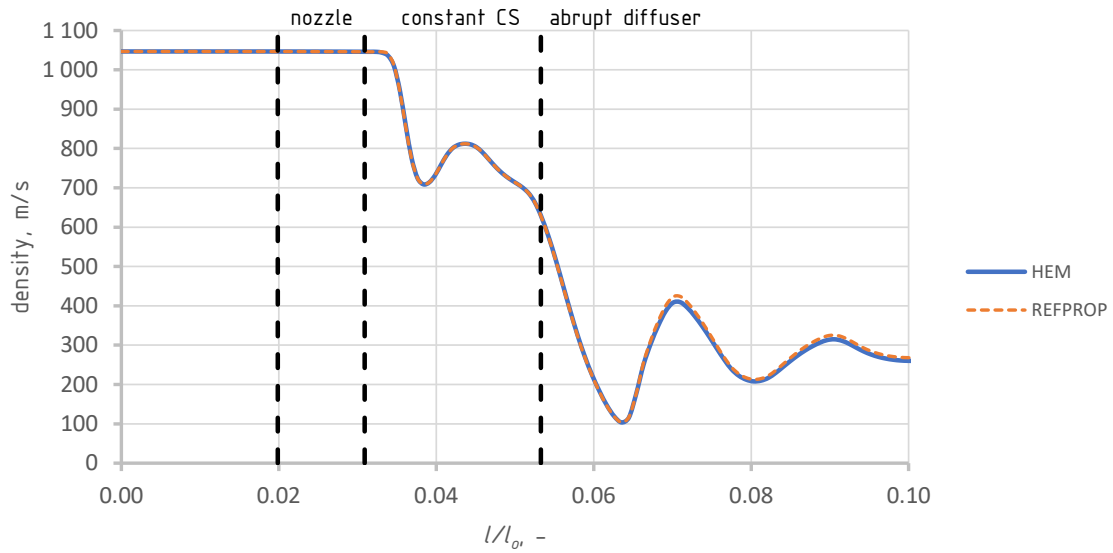


Figure 13: The axial distribution of the HEM and the REFPROP density.

664 distribution of parameters were presented to show the differences between the HEM and HRM
 665 approach.

666 The results for the HEM calculations significantly underestimated mass flow rates when com-
 667 pared to the measured results. The resulting average relative difference was 42%. This resulted

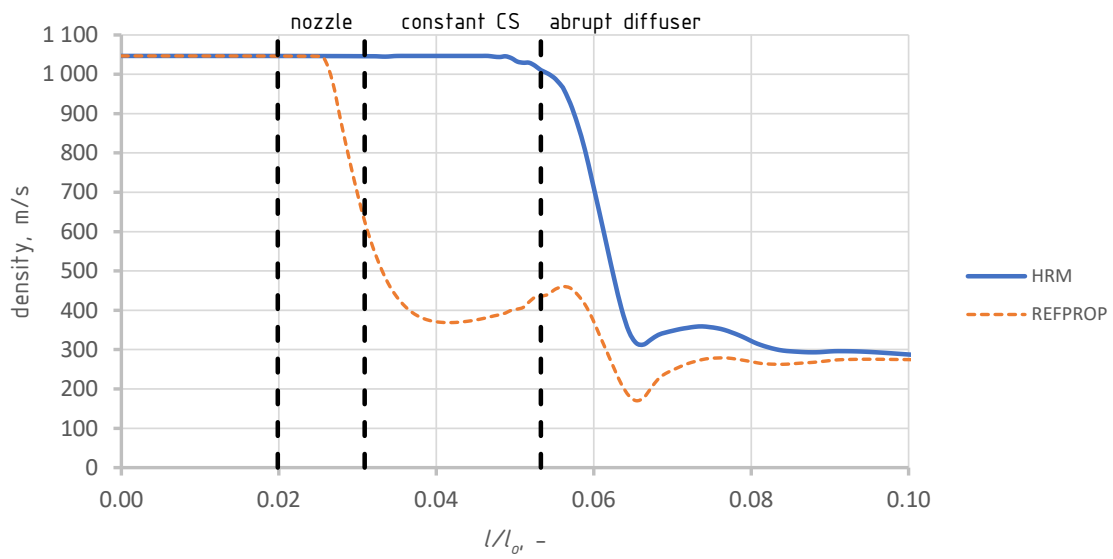


Figure 14: The axial distribution of the HRM for Variant 5 and the REFPROP density.

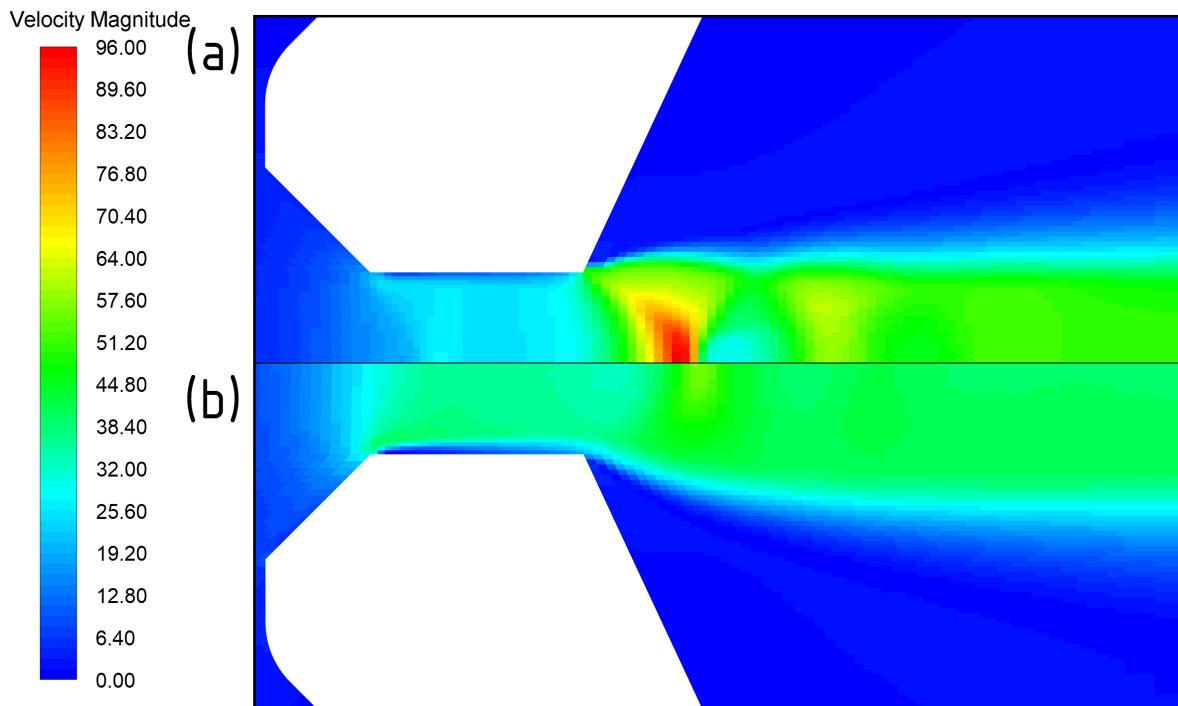


Figure 15: A comparison of the velocity in (m/s) for OP1 between (a) HEM and (b) HRM for Variant 5.

668 from the model limitations and its inability to address the sonic velocity values for the two-phase
 669 region near the liquid saturation line. This conclusion was confirmed by comparing the HEM
 670 results with analytical ones and the average difference was below 5% which is satisfactorily low.
 671 Thus, the flow for the conditions that were used, cannot be modelled using HEM because the

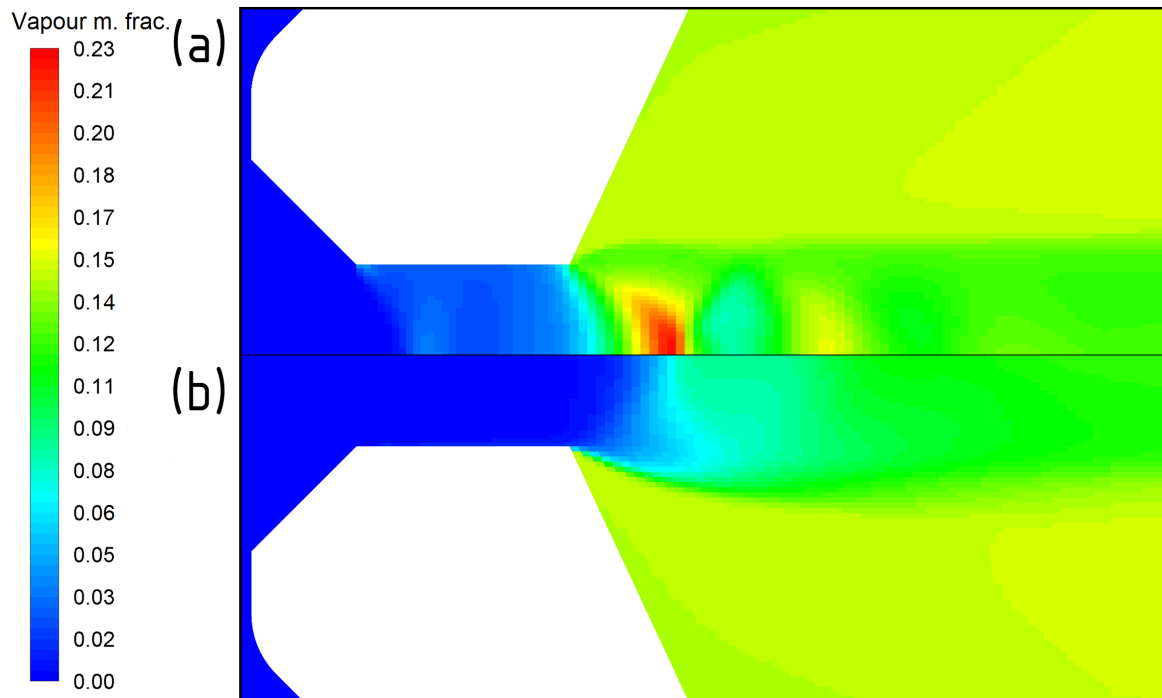


Figure 16: A comparison of the vapour mass fraction for OP1 between (a) HEM and (b) HRM for Variant 5.

672 thermodynamic non-equilibrium effects are too significant.

673 The results for HRM using water parameters from the literature, provided results with rela-
 674 tive differences of approximately 17% for the low-pressure equation parameters and 26% for the
 675 high-pressure equation parameters. The large underestimation of the MFR using the parameters
 676 of the high-pressure equation is due to the low reference relaxation time. As the higher MFR
 677 corresponds to the higher relaxation time, the reference relaxation time parameter, which was ten
 678 times higher, provided a lowered average relative difference of 8.2%. Finally, for the optimised
 679 HRM parameters, the average relative difference was approximately 5.3%. While the optimised
 680 HRM parameters determined in this study apply only to the fluid, geometry and conditions used,
 681 the methodology, which gives those parameters, can be applied to different geometries and fluids
 682 since it was successfully applied in this study and the Haida et al. (2018) study which investigated
 683 CO₂ flow through the ejector. This gives researchers the potential to adapt the HRM approach to
 684 different working fluids and this can be highly desirable for environmental reasons, e.g., HFO or
 685 natural refrigerants. Combining this with the fact that HRM can be used for different expansion
 686 devices, like an ejector, a modified HRM may be an attractive approach for modelling novel solu-
 687 tions in refrigeration from an environmental perspective. Furthermore, this is the first application
 688 of the modified HRM to an EEV simulation and the first introduction of the HRM parameters for
 689 R410, while in the literature, the HRM parameters are only available for water and CO₂. In addi-
 690 tion, the model developed can serve as a design optimisation tool for the high efficiency EEV types
 691 examined in the current study and can be useful for other types of valves such as a needle-using

692 EEV. The model design and optimisation capabilities will be increased even more in the future,
693 when a tool based on entropy generation will be implemented for the model, taking advantage of
694 CFD modelling ability to show local phenomena.

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Acronyms and abbreviations

ANN	artificial neural network
CFD	Computational Fluid Dynamics
COP	coefficient of performance
CS	cross-section
DEM	Delayed Equilibrium Model
EEV	electronic expansion valve
EoS	equation of state
EV	expansion valve
GA	genetic algorithm
GCI	Grid Convergence Index
HEM	Homogeneous Equilibrium Model
HRM	Homogeneous Relaxation Model
MFR	mass flow rate
OC	optimisation configuration
OF	objective function
OP	operating point
UDS	User-Defined Scalar

Latin letters

A	area, m^2
A_{th}	cross-section area of the throat, m^2
a	exponent of the void fraction, -
b	exponent of the non-dimensional pressure difference, -
C_1	turbulence model coefficient, -
$C_{1\epsilon}$	turbulence model coefficient, -
C_2	turbulence model coefficient, -
$C_{3\epsilon}$	turbulence model coefficient, -
C_f	discharge coefficient for incompressible liquid, -
c_p	specific heat capacity, $\text{J kg}^{-1}\text{K}^{-1}$
E	total specific enthalpy, J kg^{-1}
\dot{g}	mass flux, $\text{kg s}^{-1}\text{m}^{-2}$
G_b	generation of k due to buoyancy, $\text{kg s}^{-3}\text{m}^{-1}$
G_k	generation of k due to mean velocity gradients, $\text{kg s}^{-3}\text{m}^{-1}$
h	specific enthalpy, J kg^{-1}
j	quantity compared in the relative difference, -
k	turbulent kinetic energy, $\text{m}^2 \text{s}^{-2}$
l	length, m
l_o	total length, m
\dot{m}	mass flow rate, kg s^{-1}
N	number of mesh cells, -
p	pressure, Pa
s	specific entropy, $\text{J kg}^{-1}\text{K}^{-1}$
S	mean strain rate magnitude, s^{-1} 31
S_{ij}	mean rate-of-strain tensor, s^{-1}
T	temperature, K
t	time, s
\mathbf{u}	velocity vector, m s^{-1}
u	velocity vector component, m s^{-1}

u_x	velocity vector component perpendicular to the gravitational vector, m s^{-1}
u_y	velocity vector component parallel to the gravitational vector, m s^{-1}
x	vapour mass fraction, -
Y_M	fluctuating dilatation dissipation, $\text{kg s}^{-3}\text{m}^{-1}$

Greek Letters

α	void fraction, -
Γ	vapour generation rate, $\text{kg m}^{-3}\text{s}^{-1}$
δ	relative difference, %
ϵ	turbulent dissipation rate, m s^{-3}
η	mean strain, -
θ	relaxation time, s
θ_0	reference relaxation time, s
κ	heat capacity ratio, -
λ	thermal conductivity, $\text{W m}^{-1}\text{K}^{-1}$
μ	dynamic viscosity, $\text{kg m}^{-1}\text{s}^{-1}$
μ_{turb}	turbulent viscosity, $\text{kg m}^{-1}\text{s}^{-1}$
ν	kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
ρ	density, kg m^{-3}
σ_ϵ	turbulent Prandtl number for the turbulent dissipation rate, -
σ_k	turbulent Prandtl number for the turbulent kinetic energy rate, -
τ	stress tensor, Pa
ϕ	non-dimensional pressure difference at the relatively high pressure, -
ψ	non-dimensional pressure difference at the relatively low pressure, -

Subscripts

<i>bern</i>	Bernoulli
<i>c</i>	thermodynamic critical point
<i>cal</i>	calculations
<i>C1</i>	optimisation configuration 1
<i>C2</i>	optimisation configuration 2
<i>CPC</i>	custom parameter calculations
<i>eq</i>	equilibrium
<i>exp</i>	experimental
<i>hp</i>	high-pressure
<i>in</i>	inlet
<i>l</i>	liquid saturation line
<i>lp</i>	low-pressure
<i>min</i>	minimal
<i>ml</i>	metastable conditions
<i>o</i>	stagnation
<i>out</i>	outlet
<i>s</i>	saturation
<i>th</i>	throat
<i>turb</i>	turbulent
<i>v</i>	vapour saturation line

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