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The efficient computational tools for the design process of the transcritical two-phase ejectors for natural-based working fluids

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ABSTRACT

Natural-based working fluids for refrigeration are becoming a standard commercial solution due to the dynamic research and development in this area as well as law regulations. The state-of-the-art ejector technology for R744 systems reached current status due to a significant interest on modelling approaches and effective regulation concepts. The development path of the fast and efficient design tools based on the numerical simulations could be described as a key feature for the R744 commercial technology. In this study, one of the most effective numerical approaches dedicated for the two-phase CO2 ejector design and analysis is discussed. Namely, homogeneous equilibrium and relaxation model for high motive pressures and mixture approach for lower motive pressures were reviewed. According to the requirements of the effective design tools, the comparison also included a prediction of the vapour quality at given operating conditions and the corresponding computational costs. Moreover, several research studies on swirling and bypassing solutions as well as commercial applications of multi-ejector device and reduced order models for regulation systems where aforementioned models were used was described. Conclusions on a potential of the reviewed approaches were formulated having regard possible utilisation for the design process of the ejector based R744 systems.

1. INTRODUCTION

Advanced tools from the scope of computational fluid dynamics were described in the literature regarding its accuracy in a proper area of the operating conditions which corresponds to the phenomenon scope occurring in the ejector ducts. The path from examples of the effective 1-D (Banasiak, Hafner, & Andresen, 2012) to advanced 3-D models (Giacomelli, Mazzelli, & Milazzo, 2018; Lucas, Rusche, Schroeder, & Koehler, 2014; Palacz, Haida, et al., 2017; Yazdani, Alahyari, & Radcliff, 2012) was described regarding models features and its consequences in the mass flow rate prediction accuracy. Current development of the numerical models dedicated for the R744 ejector simulations were briefly described in the last work focused on the non-equilibrium approach (Bodys, Smolka, Palacz, Haida, & Banasiak, 2020). The authors developed model on the basis of the previously formulated homogeneous equilibrium model (HEM) approach (Smolka et al., 2013). However, the model was extended by the additional transport equation of the vapour quality with a source term responsible for a boiling phase-change during an expansion process in convergent-divergent motive nozzle (HNB).

In this study, the aforementioned HNB model development and path of the previous approaches were described regarding the potential for reliable tools in ejector shape designing process. The current models are challenged by the complex flow and high computational cost hence the novelty of the presented approach is composed of reliable, cost-effective and accurate numerical tool for the evaluation of the crucial components in R744 refrigeration cycles. The HNB model was additionally extended by source terms for cavitation modelling along 5 turbulence models were analysed and validated against the experimental data from the R744 laboratory refrigeration unit in the Silesian University of Technology (Gliwice, Poland). Crucial role of the turbulence model selection was described. Resulting accuracy and the flow analysis were presented with special concern on the effective design tools prepared for the utilisation in R744 refrigeration. Further guidance for cavitation modelling in the R744 ejectors were also proposed.

2. MODELS FORMULATION

The numerical model development could be considered as a response for the application of the ejectors and correlated operating conditions. Hence, first of the developed models called homogeneous equilibrium model (HEM) was considered for a high accuracy in high motive conditions corresponding to high ambient temperatures. Extensions of the numerical approaches regarding motive conditions were developed for lower motive pressures. Aforementioned extensions and further modifications were introduced regarding that each model should deliver results with the accuracy at the level of 10-15 % comparing to the experimental data. Moreover, criterion of low computational cost was assumed in order to maintain possibility of shape optimisation and potential for the reliable design process. Generally, the model require absolute pressure and temperature in order to provide the mass flow rate data at each ejector port which are a base for validation and evaluation of the model accuracy. The thermodynamic parameters inside the domain are described by flow relationships in a form governing equations for continuity of mass (eq. 1) and momentum (eq. 2) (Chung, 2010) as well as energy in form of specific-enthalpy (eq. 3) (Smolka et al., 2013). The description of additional features was provided below for each model type separately.

$$\nabla \cdot \left(\bar{\varrho}\tilde{\mathbf{u}}\right) = 0 \tag{1}$$

$$\nabla \cdot \left(\bar{\varrho}\tilde{\mathbf{u}}\tilde{\mathbf{u}}\right) = -\nabla\bar{p} + \nabla \cdot \tilde{\tau} \tag{2}$$

$$\nabla \cdot \left(\bar{\varrho}\tilde{\mathbf{u}}\tilde{E}\right) = \nabla \cdot \left[\left(\frac{\lambda}{\frac{\partial h}{\partial T}}\right)_p \nabla\tilde{h} - \left(\frac{\lambda}{\frac{\partial h}{\partial T}}\right)_p \left(\frac{\partial h}{\partial p}\right)_T \nabla\bar{p} + \tilde{\tau} \cdot \tilde{\mathbf{u}}\right] \tag{3}$$

2.1 Baseline approach based on the homogeneous equilibrium model

The homogeneous equilibrium model (HEM) is based on the assumption of equilibrium between both phases. In particular, it is assumed that the velocity, pressure and temperature of gaseous and liquid phase are equal. In consequence, the mechanical and thermodynamic equilibrium for both phases is defined as:

$$\begin{cases} p_l = p_g = p \\ T_l = T_g = T \\ v_l = v_g = v \end{cases} \tag{4}$$

Consequently, all the properties of the fluid can be considered as the function of pressure and specific enthalpy (Palacz et al., 2015):

$$\{\rho, \mu, k, c_p\} = f(p, h) \tag{5}$$

The HEM approach was extensively used by numerous researchers to simulate the fluid flow inside ejectors. (Smolka et al., 2013) used that model to simulate the single-phase (R134a) and two-phase ejector (R744). Similar, approach for CO_2 ejector modelling was used by (Lucas et al., 2014). Nevertheless, the mentioned authors validated the model for very limited ejector operational envelope typical for heat pump application.

The more detailed assessment of the HEM accuracy was provided by (Palacz et al., 2015). These authors analysed the HEM fidelity for the operating conditions typical for the supermarket R744 refrigeration systems. The map of the investigated ejector operating regimes is presented in Fig. 1. In addition, the discrepancy between the measured and simulated mass flow rate for the motive nozzle is presented in that figure. As it can be seen, the fidelity of the HEM for decrease significantly with the decreasing motive nozzle pressure and temperature.

(Palacz et al., 2015) concluded that HEM accuracy is acceptable for the motive nozzle operating regimes distributed above or close to the CO_2 critical point. For such operating conditions the metastable effects related to the expansion of the fluid to two-phase region are negligible. Therefore, the HEM prediction of the motive nozzle mass flow rate was satisfying, especially regarding the total computational time for single case at the level of approximately 20 minutes. On the other hand, for the motive nozzle operating conditions distributed far left from the liquid saturation curve or lower motive nozzle pressure/temperature more advance modelling approach that include the metastable effects should be employed.

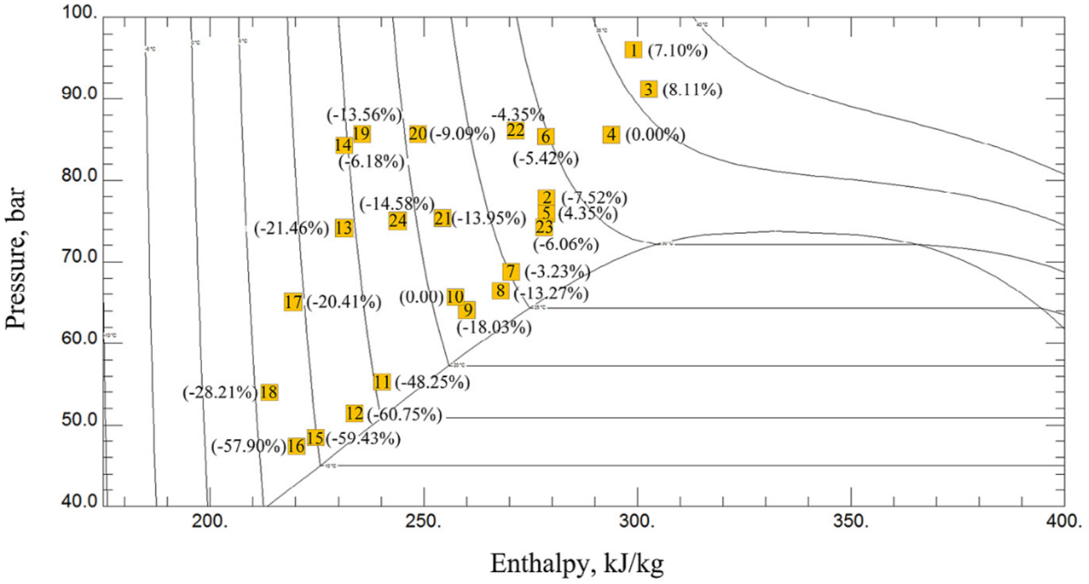

Figure 1: The motive nozzle operating regimes and discrepancy (brackets) between the measured and simulated mass flow rate for HEM (Palacz et al., 2015)

2.2 Development of the modified homogeneous relaxation model

Regarding the aforementioned metastable effect, an enhancement of the HEM approach for the R744 flow was done using homogeneous relaxation model (HRM) and modify constants defined in the relaxation time formulation. In HRM, the metastability effect of the flashed two-phase flow is taken into account. Therefore, the additional vapour mass balance equation is described in the following form (Bilicki, Kestin, & Trevor, 1990):

$$\nabla \cdot (\tilde{\rho}\tilde{x}) = -\tilde{\rho}\left(\frac{\tilde{x} - \tilde{x}_{eq}}{\tilde{\theta}}\right) \tag{6}$$

where x is the instantaneous vapour quality of the two-phase flow, x_{eq} is the vapour quality at the equilibrium state and θ is the relaxation time in s. According to Haida et al. (2018) the relaxation time for CO_2 two-phase flow is defined by the following equation:

$$\tilde{\theta} = \theta_0 \cdot \tilde{\alpha}^a \cdot \bar{\varphi}^b \begin{cases} \theta_0 = 1.0e-07 & a = 0.0 & b = 0.0 & p_{mn} = 73.77 \text{ bar} \\ \theta_0 = 9.0e-06 & a = -0.67 & b = -1.73 & 59 \text{ bar} \leq p_{mn} \leq 73.77 \text{ bar} \\ \theta_0 = 1.5e-06 & a = -0.67 & b = -2.00 & p_{mn} \leq 59 \text{ bar} \end{cases} \tag{7}$$

where θ_0, a and b are the constant relaxation time coefficient defined for different motive nozzle pressure ranges p_{mn}, α is the void fraction and φ is the non-dimensional pressure difference defined as follows:

$$\tilde{\alpha} = \frac{\tilde{x} \cdot \bar{\rho}}{\bar{\rho}_v} \tag{8}$$

$$\bar{\varphi} = \left| \frac{\bar{p}_{sat} - \bar{p}}{p_{crit} - \bar{p}_{sat}} \right| \tag{9}$$

where ρ_v is the density of the saturated vapour, p_{sat} is the saturation pressure based on the motive nozzle inlet conditions and p_{crit} is the critical pressure of CO_2.

The $k - \omega$ SST model was used to model the turbulent flow inside the ejector (Ansys, 2019). According to Mazzelli et al. (2015), the $k - \omega$ SST model showed the best agreement of the global and local flow parameters inside the ejector.

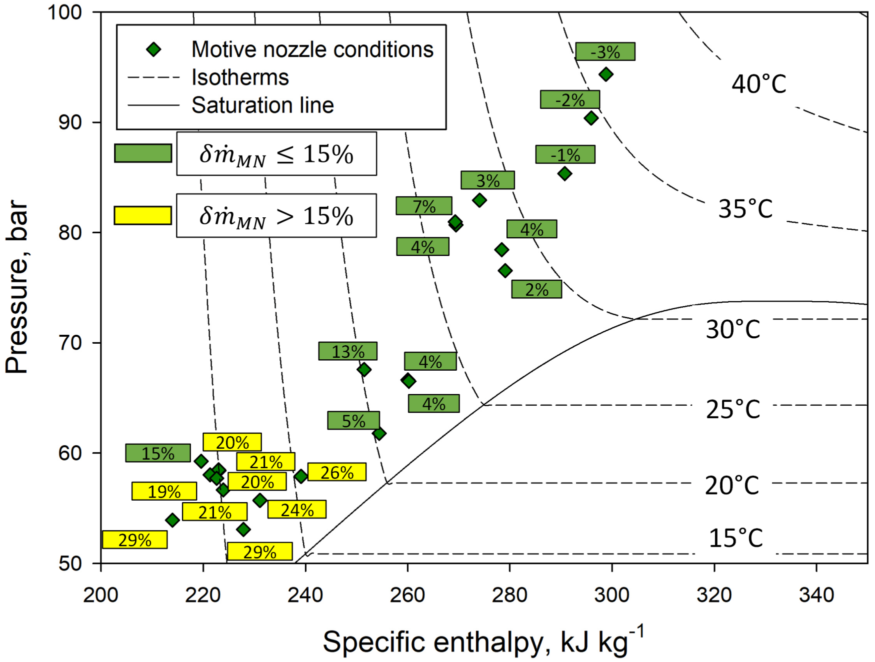

Figure 2: Motive nozzle mass flow rate discrepancy on the R744 pressure-specific enthalpy diagram obtained using modified HRM CFD model. Adapted from Haida et al. (2018).

Hence, the foregoing turbulence model was applied into the CFD model to simulate the flow behaviour inside the R744 two-phase ejector. The CFD simulations were performed in two steps. Firstly, the HEM calculations were computed. The convergence criterion was reached when the MFR imbalance was below 1% and both motive nozzle and suction nozzle MFRs were stabilised. When the HEM calculations obtained the convergence criterion, the HRM computations were performed until the similar convergence criterion was reached. In this manner, the convergence problems for all the investigated operating points were not observed. The total computational time for single case was of approximately 40 minutes.

The accuracy of the R744 two-phase ejector CFD model with modified HRM approach was shown in Fig. 2. The motive nozzle mass flow rate discrepancy was presented on the R744 pressure-specific enthalpy diagram at the selected operating points. The results obtained by the CFD model were compared in twenty one points reached during experimental investigation at the subcritical conditions, near the critical point, and the transcritical conditions. The similar accuracy of the modified HRM model was obtained above the critical point within ±10% when compared to the HEM approach. Moreover, the high accuracy within ±15% was reached by the modified HRM model above the motive nozzle pressure of 59 bar up to the critical point. Finally, the motive nozzle mass flow rate discrepancy was increased above 15% Hence, the application range of the modified HRM model was extended to the subcritical conditions up to the motive nozzle pressure of 59 bar (Haida et al., 2018).

2.3 Homogeneous non-equilibrium approach based on the boiling source (HNB)

In the last approach, the transport equation of the vapour quality used in the HRM was further modified. The source term was introduced to the right-hand side of the equation (2.2). Hence, expansion process with simultaneous non-equilibrium process of the boiling phase change was based on (Carey, 2007). The following relation for vapour mass generation rate R_{boi} was implemented to the vapour mass fraction equation:

$$R_{boi} = \pm\left[\frac{\widehat{\sigma}}{2-\widehat{\sigma}}\right]\left(\frac{M}{2\pi G_c T_{sat}}\right)^{1/2}\left[p - p_{sat}\right] \tag{10}$$

where T_{sat} is the local saturation temperature and P_v is the saturation pressure obtained for isentropic expansion from the motive nozzle inlet conditions. That approach was utilised in the study presented by (Haida et al., 2018). The coefficient is the accommodation coefficient (AC) that represents the number of molecules passing during the phase change process. The aforementioned AC needs to be adjusted according to the experimental data. Moreover, the value of that coefficient varies with the motive nozzle OC and the selected working fluid. Finally, the vapour mass fraction as the third independent parameter was used for the properties computation of the mixture quantities (Stadtke, 2006):

$$\{\rho, \mu, \lambda, c_p\} = f(p, X) \tag{11}$$

$$\rho = \frac{1}{X/\rho_g + (1-X)/\rho_l} \tag{12}$$

$$\mu = \frac{1}{X/\mu_g + (1-X)/\mu_l} \tag{13}$$

$$\lambda = \frac{1}{X/\lambda_g + (1-X)/\lambda_l} \tag{14}$$

$$c_p = \frac{1}{X/c_{p,g} + (1-X)/c_{p,l}} \tag{15}$$

Calibration procedure of the accommodation coefficients were based on the experimental data obtained for two ejectors of different size (Bodys et al., 2020). The operating conditions of the motive nozzle port was presented along the aforementioned coefficients in Fig. 3. Moreover, the suction nozzle pressure and temperature was maintained at the level of 28 bar and 4^{o}C. Finally, the pressure lift was from the range of 2-3 bar. Hence, the boundary conditions of the suction and outlet port varied negligibly while the motive nozzle conditions were considered as a variable. The criterion for each coefficient was motive mass flow rate accuracy below 1 %. Resulting coefficients were transformed into the approximation function in order to cover the motive pressures in full and continuous manner. The function uses absolute pressure and specific enthalpy at the motive port in order to calculate value of the accommodation coefficient. Final accuracy of the motive nozzle mass flow rate prediction using the approximation function was below 12.5 % as presented in Fig. 4. Having regard that model was implemented to the ejectorPL platform (Palacz, Smolka, Nowak, Banasiak, & Hafner, 2017), the simulation time is about 45 minutes. In a consequence this approach could be utilised in effective way for other fluids and ejector geometries. Resulting model would be a valuable for reduced order models derivation and further system computations.

Unfortunately, high accuracy of the motive nozzle mass flow rate was not related with the same level of suction nozzle mass flow rate presented in Fig. 5. For the higher motive pressure obtained accuracy was below 20 % considering $k-\omega$-SST. However, lower motive pressures definitely need more development cause this turbulence model was not reliable anymore.

2.4 Extension of HNB approach by cavitation source and turbulence model screening

The extension of the HNB approach was introduced in a form of a cavitation modelling. The phase change related with this phenomenon was based on the approach presented by (Singhal, Athavale, Li, & Jiang, 2002) in equation (2.4). Hence, additional source term was implemented to the transport equation of the vapour mass fraction. In similar to the source term correlated with the boiling phase change, the cavitation source term requires empirical assessment of the coefficient which directly indicates the intensity of the vapour phase generation rate. Validation was proceeded within 12 operating points obtained at the laboratory R744 test rig equipped in the ejector dedicated to the visualisation research (Haida et al., 2020). The motive pressure between 50 bar and 70 bar allowed for the assessment of the aforementioned formulation.

$$R_{cav} = \kappa \frac{\sqrt{k}}{\zeta} \rho_l \rho_v \left[\frac{2}{3} \frac{p_v - p}{\rho_l} \right]^{1/2} (1-X) \tag{16}$$

where R_{cav} is the cavitation source term, ζ is a surface tension and κ is a cavitation constant. Regarding variable temperature within the flow, the surface tension was computed on the basis of formulation adapted from a study delivered by (Muratov & Skripov, 1982):

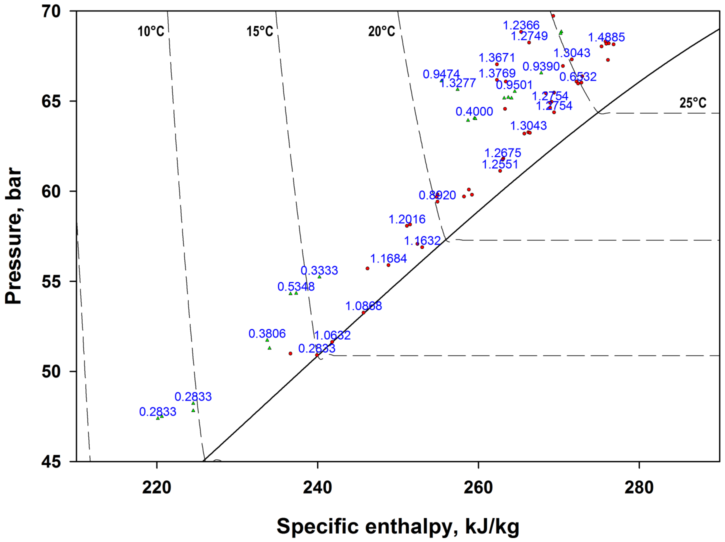

Figure 3: Calibrated accommodation coefficients in function of the motive pressure and specific enthalpy

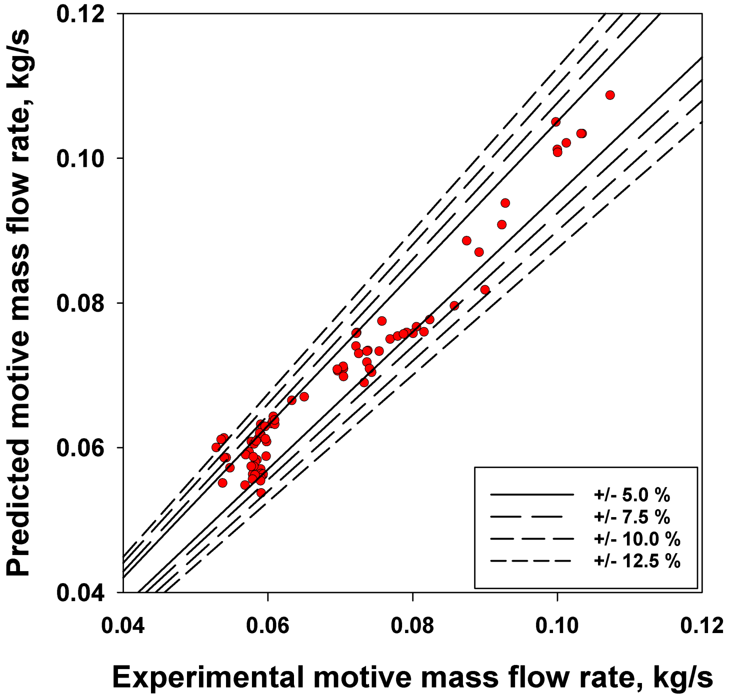

Figure 4: Accuracy dispersion of the motive nozzle mass flow rate prediction

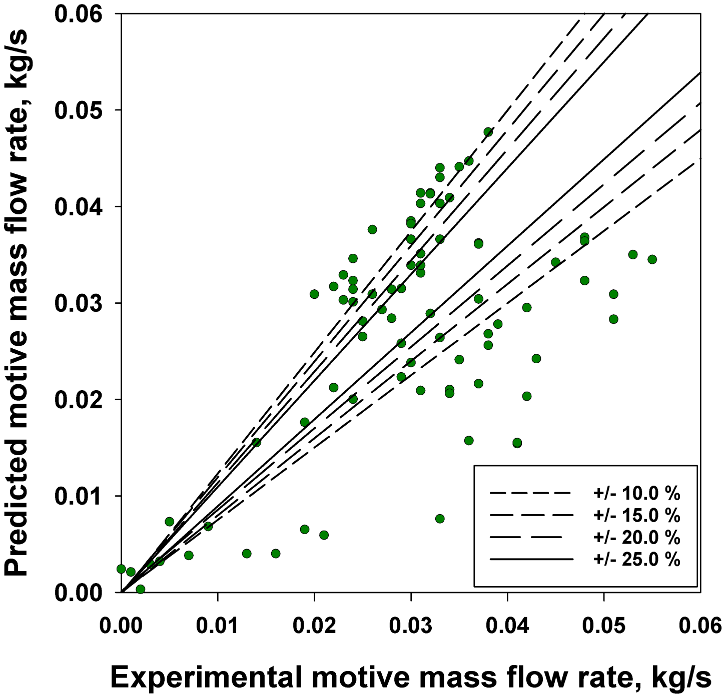

Figure 5: Accuracy dispersion of the suction nozzle mass flow rate prediction

$$\zeta = (0.0597 \cdot T^2) - (1.5546 \cdot T) + 10.172 \tag{17}$$

The constant κ should be adjusted for the considered working fluid and the flow conditions in order to provide proper mass flow rate and flow pattern (Singhal et al., 2002). In this study several intensities of the cavitation phenomenon was tested trough various values of the cavitation constant κ. Finally, the constant κ equal to 1 and 6 were concerned on the basis of the results analysis related with the given constant. Introduced cavitation phenomena was related with intensified evaporation during the expansion process. Finally, the aforementioned source term was introduced to the final form of the vapour mass fraction transport equation:

$$\nabla \cdot \left(\tilde{\rho}\tilde{\mathbf{u}}\tilde{X}\right) = R_{boi} + R_{cav} \tag{18}$$

Parallel to the cavitation, turbulence models were considered since its presence is of high importance in the pre-mixer chamber as well. Aforementioned two cavitation constants were considered for the twelve boundary conditions and five turbulence models. The results were presented in Fig. 6 using decreasing motive port conditions with increasing number of the boundary condition. The colours of the motive nozzle markers were presented with blue scale while the suction nozzle with the brown scale. The motive nozzle markers oscillated between plus minus 10 %. The suction nozzle markers are more dispersed with over-prediction for higher pressures and under-prediction for lower motive pressures. Preliminary analysis revealed the aforementioned trend where most of the suction nozzle markers in the higher motive pressures indicated overestimation. Differently with the lower pressures. Moreover, the highest changes between cavitation constant were computed for $k-\varepsilon$ Standard. Regarding the accuracy, $k-\omega$ SST model should be used for higher pressures and $k-\varepsilon$ Standard for the lower values of the motive pressure. These approach should provide the accuracy of the suction mass flow rate on the level of 20 %.

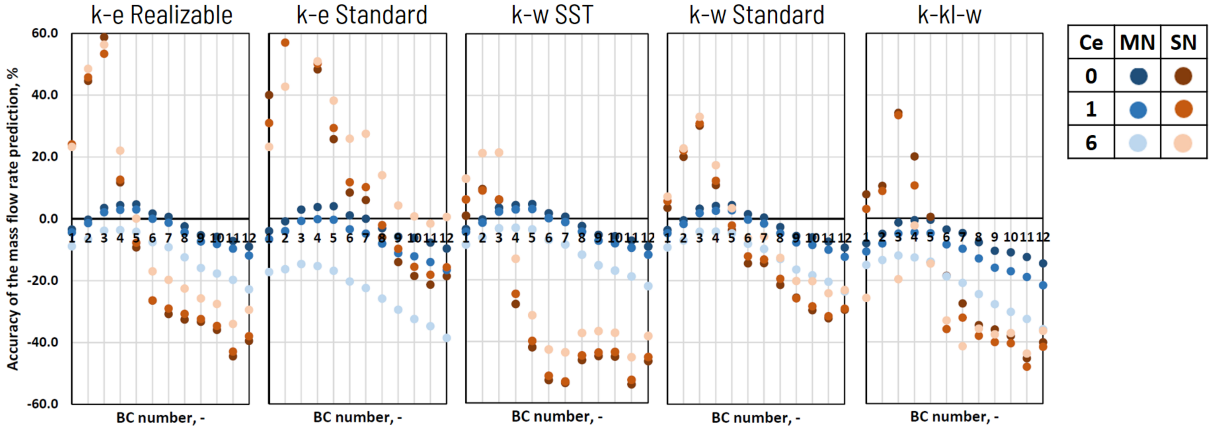

Figure 6: Results of the turbulence and cavitation screening regarding accuracy of the mass flow rate prediction

3. CONCLUSIONS

The accuracy of the mass flow rate prediction could be treated as a key parameter of the models evaluation. However, the high accuracy of the motive nozzle mass flow rate prediction is not necessary correlated with the high accuracy of the suction flow prediction. The reliable design tools for ejectors shapes should be able to predict both of the streams due to high importance of both streams in further system analysis and components selection.

Another key feature regarding models usability is the computational cost. In the considered approaches approximately 45 minutes of the simulation was ensured for each operating point. This time should be treated as a satisfactory regarding the models simplicity and utilised computing power.

Regarding the applicability of HEM and HRM approaches, an acceptable prediction quality was obtained. In the case of HNB approach further improvement should be provided due to low accuracy of the suction nozzle mass flow rate prediction. Namely, other ejector geometries for high and low-pressure lifts will be analysed, the cavitation source term defined by other authors will be evaluated as well. Finally, full 3D analysis of the flow in the pre-mixing chamber should be considered as next crucial factor which could provide higher accuracy with consequence of the higher computational costs.

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