A comparison of homogeneous equilibrium and relaxation model for CO$_2$ expansion inside the two-phase ejector

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Abstract. In this study, the comparison of the accuracy of the homogeneous equilibrium model (HEM) and homogeneous relaxation model (HRM) is presented. Both models were applied to simulate the CO$_2$ expansion inside the two-phase ejectors. Moreover, the mentioned models were implemented in the robust and efficient computational tool ejectorPL. That tool guarantees the fully automated computational process and the repeatable computations for the various ejector shapes and operating conditions. The simulated motive nozzle mass flow rates were compared to the experimentally measured mass flow rates. That comparison was made for both, HEM and HRM. The results showed the unsatisfying fidelity of the HEM for the operating regimes far from the carbon dioxide critical point. On the other hand, the HRM accuracy for such conditions was slightly higher. The approach presented in this paper, showed the limitation of applicability of both two-phase models for the expansion phenomena inside the ejectors.

1. Introduction

The throttling losses have the significant influence on the refrigeration or heat pump system performance [1]. In particular, that losses are very high for the high pressure refrigeration systems, i.e. carbon dioxide refrigeration systems. The application of the ejectors in such systems improves the coefficient of performance (COP) of such systems [2, 3, 4, 5]. In addition, the simplicity of the device (e.g. no moving parts) makes ejectors cheaper and more reliable comparing to e.g. expanders. Nevertheless, the performance of the ejector and in consequence the mentioned COP improvement, depends on the ejector design. Hence, the numerous of mathematical models were developed to numerically investigate the ejector performance.

To model the fluid flow inside the ejector various mathematical formulations are presented in the literature. The available models vary from relatively simple 1-D models to the complex 3-D CFD models. Nevertheless the accuracy of the model mostly depends on the two-phase flow model. Banasiak and Hanfer [6] used 1-D model to assess the ejector performance for given operating conditions. In that model the two-phase flow was modelled using delayed equilibrium model (DEM) enhanced with homogeneous nucleation theory (NHT). Unfortunately, to better understand the flow of the refrigerant inside the ejector (e.g. turbulence intensity field) more complex model were desired.

The 3-D computational model was introduced by Smolka et al. [7]. In this approach, the two-phase flow was modelled with the HEM. Moreover, the NIST REFPROP [8] libraries were implemented to the model to obtain the real fluid properties. Similar approach was used in the
analysis performed by Lucas et al. [9], however the computational domain was reduced to 2-D axisymmetric. In both cases, the application of the HEM provided the acceptable accuracy of the model prediction. However, in both mentioned papers the model performance was assessed for relatively high operation pressures and temperatures close to the critical point of CO$_2$.

The authors of [10] analysed the performance of the HEM for wide range of the operating conditions, typical for supermarket refrigeration system. Moreover, the mathematical model was implemented in the in-house developed computational tool named ejectorPL. The model accuracy was evaluated by the comparison of the measured and computed mass flow rates. The measured mass flow rate were captured during the experimental campaign of the considered ejectors in SINTEF Energy, Trondheim, Noraway [11]. The analysis results showed that fidelity of the solution decrease significantly for the operating regimes far from the critical point. The lack of the model accuracy for such operating regimes is caused by the neglecting the metastable effects in HEM approach. On the other hand, that effects are considered in homogeneous relaxation model [12, 13, 14]. The relaxation time included in that model take into account the delay of the phase change during the expansion in the metastable regions. Unfortunately, to the best knowledge of the authors the analysis of the HRM accuracy similar to [10] was not performed yet. Therefore, the accuracy of that model was evaluated in this paper and then compared to the HEM accuracy.

2. Mathematical model

As it was mentioned in previous section the homogeneous equilibrium and relaxation models were used to simulate the fluid flow inside the ejector. Originally, the approach used by [7] with the HEM for two-phase flow was used to evaluate the HEM accuracy. Then the HRM was implemented to that model. The turbulence was modelled with the Realisable $k – \epsilon$ model and external NIST REFPROP [8] libraries were used to obtain the real fluid properties. Moreover, the ejectorPL [10, 15] computational tool was used for the computations. That tool guaranteed the consistent computational procedure for both, HEM and HRM, for any give operating conditions or ejector shape. The ejectorPL is the in-house developed script which combines the commercial Ansys packages such as: Ansys ICEM CFD and Ansys Fluent. The schematic view of ejectorPL is presented in Fig. 1. In addition, the dedicated

![Diagram](image.png)

**Figure 1.** The schematic view of the ejectorPL software
initialization procedure was developed to reduce the computational time. The numerical grids used for the computations were composed by approx. 10000 cells to guarantee the mesh-independent results.

2.1. HEM formulation

The homogeneous equilibrium model is one of the simplest approaches that can be used to model two-phase flow. In this model, the mechanical and thermodynamic equilibrium between liquid and vapour phase is assumed. The mass, momentum and energy equation for the steady state HEM are described by the following form:

\[ \nabla \cdot (\rho \mathbf{U}) = 0 \]  
\[ \nabla \cdot (\rho \mathbf{UU}) = -\nabla p + \nabla \cdot \tau \]  
\[ \nabla \cdot (\rho \mathbf{UE}) = \nabla \cdot (k \nabla T + \tau \cdot \mathbf{U}) \]

where the \( \rho \), \( p \), \( \mathbf{U} \), \( T \), \( \tau \), \( k \) and \( E \) stand for the density, pressure, velocity vector, temperature, stress tensor, effective thermal conductivity and total enthalpy, respectively. The total enthalpy of the fluid \( E \) is defined as the sum of the specific enthalpy \( h \) of the fluid and its kinetic energy:

\[ E = h + \frac{U^2}{2} \]

The \( U \) in the equation above stands for the fluid velocity. In consequence, in HEM the transport properties of the fluid are the function of the total enthalpy and the pressure:

\[ \{\rho, c_p, k, \mu\} = f(p, h) \]

2.2. HRM formulation

In the homogeneous relaxation model, the mechanical equilibrium is assumed similar to HEM, however the non-equilibrium phase change is accounted by the relaxation thermodynamic equilibrium. That non-equilibrium phenomena the equation for the vapour mass fraction \([12, 14, 16]\)

\[ \frac{\partial (\rho \bar{x})}{\partial z} = \rho \frac{\bar{x} - x}{\theta} \]

the \( \bar{x} \) is the equilibrium vapour quality (calculated for HEM), \( x \) is actual vapour quality and \( \theta \) is the relaxation time. The \( \theta \) can be defined as:

\[ \theta = \theta_0 a^a b^b \]

where:

\[ a = \left| \frac{p_{sat} - p}{p_c - p_{sat}} \right| \]

\[ b = \frac{\rho_{sat} - \rho}{\rho_{sl} - \rho_{sv}} \]

The subscripts \( sat \), \( c \), \( sl \), \( sv \) stand for saturation conditions, critical conditions, saturated liquid and saturated vapour, respectively. The coefficients \( \theta_0 \), \( a \) and \( b \) for \( CO_2 \) were experimentally determined by Angielczyk [17]. In consequence, the Eq. (7) can be rewritten in following form:

\[ \theta = 2.15 \times 10^{-7} a^{-0.54} b^{1.76} \]

Taking into account the actual vapour quality \( x \) instead of the equilibrium vapour quality \( \bar{x} \) the mixture density need to be recalculated (Eq. 11).

\[ \frac{1}{\rho} = \frac{x}{\rho_{sv}} + \frac{1-x}{\rho_m(p, h_{ml})} \]
Subscript $ml$ in the equation above stands for the metastable liquid. Moreover, the mixture specific enthalpy needs to be recalculated, taking $x$ for account:

$$h = xh_{sv}(p) + (1 - x)h_{ml}$$  \hspace{1cm} (12)

Consequently, in HRM approach the properties of the two-phase mixture are function of pressure and actual vapour quality.

$$\{p, c_p, k, \mu\} = f(p, x)$$  \hspace{1cm} (13)

3. HEM and HRM performance

The accuracy of the considered two-phase flow models was evaluated by the comparison of the computed mass flow rates with the measured ones. The range of operating conditions used to assess the models fidelity were typical for the supermarket refrigeration system placed in the Northern and Southern Europe [18]. Moreover, the ejectors installed in that systems were experimentally analysed in the SINTEF Energy laboratory [11]. The motive nozzle operating conditions (OCs) are listed in Table 1. As it can be see, the range of the considered operating conditions vary from the OCs close and far from the CO$_2$ critical point.

In similar to, the [10] it was assumed that the model prediction is accurate if the relative difference ($\delta$) between the measured and computed value (defined in Eq.) was $\pm$ 10%.

$$\delta = \left(1 - \frac{\dot{m}_{CFD}}{\dot{m}_{EXP}}\right) \times 100$$  \hspace{1cm} (14)

The subscripts $CFD$ and $EXP$ in the equation above stand for computed value and measured value, respectively. The $\dot{m}$ is the mass flow rate.

4. Results

The motive nozzle mass flow rates were computed within the HEM and HRM approach for the OCs presented in Table 1. Then the relative difference between the measured and computed motive nozzle mass flow rates was calculated. Moreover, the discrepancy between the experimental and the computational mass entrainment ratio ($\chi$) was analysed. relative difference between the measured and computed ejector performance parameter, called mass entrainment ratio ($\chi$), was calculated. $\chi$ is defined as the ratio between the suction nozzle mass flow rate and motive nozzle mass flow rate (Eq. 15).

$$\chi = \frac{\dot{m}_{SN}}{\dot{m}_{MN}}$$  \hspace{1cm} (15)

The correct prediction of the $\chi$ is very important from the ejector efficiency point of view.

The results of the HEM and HRM accuracy analysis are listed in Table 2. Analysing the presented results it is noticeable that operating conditions distributed close to the critical point (OCs #3 and #4).
Table 2. Operating condition taken into account during the model accuracy assessment

| OCs | \( \dot{m}_{MN}, \text{kg/s} \) | \( \chi \), - | \( \delta_{\dot{m}_{MN}}, \% \) | \( \delta_{\chi}, \% \) |
|-----|-------------------------------|-----------------|-----------------|-----------------|
| 1   | 0.099                         | 0.076           | 0.079           | 0.03            | 0.00            | 0.03            | 23.23          | 20.20           | 100.00          | 0.00            |
| 2   | 0.072                         | 0.061           | 0.063           | 0.19            | 0.21            | 0.22            | 15.97          | 11.96           | -10.52          | -15.79          |
| 3   | 0.067                         | 0.066           | 0.069           | 0.41            | 0.42            | 0.38            | 1.49           | -3.90           | -2.43           | 7.31            |
| 4   | 0.079                         | 0.079           | 0.083           | 0.41            | 0.40            | 0.36            | -0.31          | -4.83           | 2.43            | 12.19           |
| 5   | 0.094                         | 0.094           | 0.095           | 0.34            | 0.34            | 0.36            | 0.29           | -0.80           | 0.00            | -5.88           |

The discrepancy for that points is lower than 5%, for both models. Moreover, the point #5 which was above the critical point showed good agreement with the experimental data. Nevertheless, for such conditions the HEM approach was more accurate than HRM. On the other hand, the accuracy for the low pressure points (#1 and #2) was slightly improved. It is also noticeable that the \( \chi \) prediction for the low pressure and temperature operating conditions was better for HRM. Unfortunately, considering that the \( \delta_{\dot{m}_{MN}} \) was significant for the operating conditions #1, #2 and #3 and error for \( \chi \) was small, the suction nozzle mass flow rate was incorrectly predicted. Moreover, as it can be see in Table 2, the HRM outperform the HEM or the operating conditions for which metastable effects during the phase change play significant role. However, for the operating conditions for which metastability can be neglected the HEM accuracy was higher.

Comparing the results for HEM and HRM it noticeable that the accuracy improvement of HRM is rather unsatisfying. That small difference between the models accuracy is possible caused by the incorrect formulation for \( \theta \), see Eq. (7). The experimentally assessed coefficient in Eq. (7) were determined during the experimental investigation of the converging-diverging nozzle. However, the operating conditions used for this assessment were relatively near critical point of \( \text{CO}_2 \).

5. Conclusion

The comparison of the different two-phase models were presented in this study, namely homogeneous equilibrium model and homogeneous relaxation model. To evaluate the accuracy of the models the numerical results were compared with the experimental data. That analysis was performed using the efficient computational tool called ejectorPL. The experimental data were provided by the SINTEF Energy Research, where considered ejectors were experimentally tested.

The accuracy analysis showed the limitation of the HEM. That approach should be used only for the motive nozzle operating conditions near critical point of the carbon dioxide. The decrease of the motive nozzle inlet pressure or temperature results in rapid decrease of model accuracy. However, for the points close to the critical point the HEM accuracy can be higher than HRM.

The HRM fidelity was slightly better for the low pressure or temperature motive nozzle operating conditions. Nevertheless, the improvement of the accuracy comparing to HEM was negligible. The incorrectly adjusted \( \theta \) for the considered operating conditions may be the cause of that rather small accuracy increase. Thereby, further work should be conducted to investigate the HRM results quality for the various \( \theta \) formulations.

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