Lumped parameter modelling of two-phase ejectors: numerical implications of the equilibrium assumptions

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Abstract. The use of carbon dioxide as refrigerant is attracting a growing attention and is a cutting-edge research topic. In spite of its many advantages, carbon dioxide has a major shortcoming, viz., low critical temperature. Owing to the low critical temperature, carbon dioxide cycles encompass both the sub-critical and the trans-critical operation conditions; the trans-critical operating conditions are characterized by high thermodynamic losses, requiring particular attention in the integrated component/system design criteria. In this perspective, in recent years, ejector technology has been widely recognized as a promising technical solution to support the deployment of carbon dioxide cycles, by reducing throttling losses. Unfortunately, the large variation in system operations as well as the changes in sub-critical and trans-critical operating conditions makes the numerical simulation of carbon dioxide ejector-based system a cutting-edge challenge. This paper contributes to the present day discussion on the validation of lumped parameter models for carbon dioxide ejectors. A model taken from the literature has been tested against literature data and the equilibrium assumptions, underlying the modelling approach have been tested.

1. Introduction
It is widely accepted that, in the forthcoming decades, the use of natural refrigerants will largely increase, also taking into account the recent regulations regarding [1-3]. In the broader framework of natural refrigerants, carbon dioxide is attracting a growing attention because of its many advantages [4]: beside being no-toxic it has unique properties, e.g., at given saturation temperature and pressure, the surface tension, the liquid viscosity and ratio of liquid to vapour density of carbon dioxide are the smallest compared with other refrigerants. In spite of these advantages, carbon dioxide has a major shortcoming, viz., low critical temperature (304.25 K). Thus, carbon dioxide cycles encompass the sub-critical and the trans-critical operation conditions: on one hand, sub-critical performances are valuable; on the other hand the trans-critical operating conditions are characterized by high thermodynamic losses. To reduce these losses, particular attention in the integrated component/system design is requested. For this reason, ejector technology has been widely accepted as a promising to support the deployment of carbon dioxide cycles. Ejectors provide a combined effect of compression, mixing and entrainment, with no-moving parts, structural simplicity, low capital cost, reliability, little maintenance, low initial and running cost and long lifespan [5]. Nevertheless, the efficiency of the whole system is highly influenced by the local ejector performances, which significantly depends on the geometry and operating conditions. In addition, in the case of carbon dioxide cycles, the large variation in the system operation as well as the changes in sub-critical and trans-critical operations make the numerical simulation of carbon dioxide ejector-based system a cutting-edge challenge [5]. This paper contributes to the existing discussion regarding lumped parameter models for carbon dioxide ejectors and is intended to provide guidelines for lumped parameter simulations of carbon dioxide ejectors.
2. Methods
Cardemil and Colle [6] presented a lumped parameter model, which considers ideal/real gasses and dry/wet fluids. The validation of this model for single-phase flows has been presented by Besagni et al. [7], whereas this paper focuses on the two-phase (carbon dioxide) ejectors.

First, the performances of this model are clarified in the first section of the results. In particular, the model has been tested against the experimental data of Xu et al. [8]. With regard to the calculation of the thermodynamic properties of the working fluids, the open-source thermophysical property library name CoolProp [9] was used. The effectiveness of the model is evaluated in terms of the relative error $E_R$:

$$E_R(X) = \left| \frac{X_{\text{mod}} - X_{\text{exp}}}{X_{\text{exp}}} \right| \times 100$$

where $X_{\text{exp}}$ and $X_{\text{mod}}$ are the measurement and the model estimates, respectively.

Second, the numerical implications of the equilibrium assumptions within for the calculation of the speed of sound are studied. Indeed, the chocking phenomenon that occurs in the two-phase flow is analyzed considering a model for the calculation of the speed of sound. In this case, the pressure and the temperature are not independent, but are related by means of the equation of equilibrium between the phases. Cardemil and Colle [6] suggested the use of the phase transfer relaxation model, developed by Lund and Flatten [10]. This model considers a hierarchy of hyperbolic relaxation models describing two-phase flows in pipelines; the hierarchy is characterized by the number of equilibrium assumptions imposed:

1. pressure equilibrium ($p$);
2. temperature equilibrium ($p$, $T$);
3. phase transfer equilibrium ($p$, $T$, $\mu$).

The relaxation two-phase flow model consists of six equations: the momentum conservation equation, the volume advection equation and the mass and energy conservation equations for each phase. It is possible to derive the wave velocity applying the eigenvalues analysis on this system of equations (for further information, please refer to ref.s [10, 11]). In the present implementation, each new level $n$ of equilibrium conditions added, the mixture sound velocity can be expressed as:

$$\hat{c}_{n+1}^2 = \hat{c}_n^2 + S_n$$

where $S_n$ can be written as a positive sum of squares.

3. Results
First, our results (against the experimental data of Xu et al. [8]) have been also compared with the original model results (Figure 1 and Table 1). This outcomes is a clear extension of our previous paper [7].

![Figure 1](image-url)  
(a) Experimental data from Xu et al. [8].

(b) Relative frequency distribution of the errors.

**Figure 1.** Comparison of calculated results to experimental data and distribution of the relative errors for the entrainment ratio ($\omega$).
Table 1. Efficiencies assumed and errors of the simulations against benchmark in ref. [8].

| Fluid          | Cardemil and Colle [6] | This paper |
|---------------|------------------------|------------|
| Nozzle efficiency | 0.95                  | 0.95       |
| Mixing efficiency   | 0.95                  | 0.95       |
| Diffuser efficiency  | 0.95                  | 0.95       |
| $\phi_m$         | 1                      | 1          |
| $E_R\left(\phi\right)$ [%] |                      |            |
| Min       | 0.60                  | 3.38       |
| Max       | 2.48                  | 13.78      |
| Mean      | 1.42                  | 8.04       |
| Variance  | 0.40                  | 10.98      |

The results, in terms of prediction of the entrainment ratio $\omega$, are a little different (and quite higher) compared with those of Cardemil and Colle [6]. This difference can be imputed to the numerical implementation of the two-phase speed of sound, as discussed in the following. In general, the range of applications of this model even covers two-phase flow regimes and thus it appears to represent an improvement in ejector modelling (i.e., see the validation of this model against single phase flows in ref. [7]). However, as Cardemil and Colle [6] themselves recognize, the interaction between the primary and secondary flows is not completely describable because the oblique shock and other phenomena are impossible to model through a one-dimensional analysis. Further fluid dynamics information can only be obtained through CFD simulations [5]. Anyhow, a numeric solver is required, due to the non-linear system of equations of which the model is constituted. Second, as mentioned above, a separate discussion is devoted to the relaxation two-phase model and its equilibrium assumptions. As already mentioned, the relaxation two-phase flow model [10], on which the lumped parameter model relies, is based on three equilibrium conditions. The model proposed by Cardemil and Colle [6] considers that both the pressure and the temperature are at equilibrium, but not the chemical potential of the phases. Hence, the two-phase speed of sound calculation takes on a simplified form. According to the authors, we also have relied on the same assumption. Thereby, several problems have been encountered. Indeed, the integration of the simplified two-phase model flow and the thermodynamic model has not led to convergence. The reason seems to lie in the fact that the speed of sound is underestimated and this causes problems in the resolution of the non-linear system of equations of the lumped parameter model. Thus, we implemented the two-phase model assuming the temperature, pressure and chemical potential equilibrium of the phases. Please note that the choice was dictated by numerical reasons and not for physical considerations. In this way, we were able to carry out our simulations. However, it was still necessary resort to numerical techniques, like the under relaxation method, to ensure numerical stability, but penalizing the rate of convergence. In particular, the use of under relaxation factor has been necessary in the calculation of the speed of sound at the nozzle throat, as in the following formula:

$$c_t = c_{t,old} + \alpha (c_{t,calc} - c_{t,old})$$

(3)

The relaxation factor $\alpha$ is assumed equal to 0.8. The Figure 2 shows an example of the relative error and speed of sound trends during the simulation for a determined operating condition. In particular, the Figure 2a illustrates the case of the single-phase model with R141b (discussed in ref. [7]): it has not convergence or stability problem. Figure 2b shows the result of the implementation of the two-phase model using the under relaxation factor. It may be note that in the latter case the function trends are however more discontinuous.

4. Conclusions, outcomes and outlooks
This paper contributes to the present day discussion on the validation of lumped parameter models for carbon dioxide ejectors. The model of Cardemil and Colle [6] has been tested against literature data [8] and the equilibrium assumptions, underlying the modelling approach have been tested; in conclusion, the validation proposed in our previous paper [7] is here extended for two phase flows. In addition, numerical implications of the equilibrium assumptions for two-phase speed of sound calculation are analized. In the future, it would be interesting to enquire if the use of the $p, T, \mu$ equilibrium assumption has also a physical meaning.
Figure 2. Relative error and speed of sound trends during the numerical simulation. a) single-phase model; b) two-phase model with under relaxation factor.

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