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COMPARATIVE STUDY OF R744 EJECTOR CFD MODELS

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ABSTRACT

This work presents a comparative study of four different R744 ejector CFD models at a wide range of operating conditions. The models compared are the homogeneous equilibrium model, the UDRGM mixture model, a homogeneous relaxation model and a Eulerian two-fluid model. The results are also compared to experimental data available in the literature. The models are tested for high and low operating pressures, and the effects of non-equilibrium are discussed. The results are discussed and recommendations for model developments are suggested.

Keywords: Refrigeration, Carbon Dioxide, Compressors, COP, Evaporators, Energy Efficiency

1. INTRODUCTION

In recent years, the HVAC&R industry is turning away from high global warming potential gases (GWP) refrigerants, such as the hydroflourocarbon (HFCs) gases, and increasingly toward natural and environmentally friendly refrigerants. One of the primary candidates for many HVAC&R applications is using R744 (CO_2) as a refrigerant. R744 boasts high system efficiency, low refrigerant cost, non-toxicity, non-flammability, aswell as negligible GWP. Many technologies for R744 systems have been developed over the last decades, especially for high ambient temperature applications. Of these technologies, special interest has been devoted to two-phase ejectors. A two-phase R744 ejectors is a work recovery device that uses the throttling losses inherent in the process to recompress a secondary flow to a higher pressure. Still, the design process for of these devices is not yet developed due to the complex nature of the flow. Therefore, design and modelling tools using computational fluid dynamics (CFD) has been a focal point of research over the last decade.

Several models have been presented in the literature, all with different benefits and drawbacks. The most commonly employed model is the Homogeneous Equilibrium Model (HEM) (Smolka et al., 2013, Palacz et al., 2015). This approach assumes full equilibrium in momentum, temperature and pressure between the phases. This approach is simple, yet efficient for modelling many ejector functions. However, it was later found that this approach loses accuracy when operating conditions at below critical pressure are considered (Palacz et al., 2017). This is illustrated in Figure 1., where motive nozzle mass flow rate accuracy is visually presented in a P-h diagram. Several novel models that account for this thermodynamic non-equilibrium has since then been presented. A homogeneous relaxation model (HRM) was proposed by Palacz et al. (2017). This approach was later extended with variable relaxation scales to achieve better accuracy at a wide range of operating conditions (Haida et al., 2018). Later Giacomelli et al. (2018,2019) presented a mixture model, which uses sub-models for evaporation and condensation to account for the relaxation process to equilibrium conditions. This approach showed better accuracy than previous approaches, however this came at the cost of very high computational costs. Recently, (Bodys et al., 2020) presented a mixture model for very low pressure conditions. Recently, Ringstad and Hafner (2020), proposed using a more complex two-fluid CFD model. This approach is still under development as is dependent on many more sub-model parameters than previous models. While many of these advances has improved the modelling capabilities for R744 two-phase ejectors, siginificant errors are still observed when comparing with experiments.

This paper will present a comparison of a HEM, a HRM, a mixture model by Giacomelli et al. (2018) and a Eulerian-Eulerian (two-fluid) non-equilibrium model. For more details on R744 ejector models, see the detailed

review of the state of the art R744 ejector models (Ringstad et al., 2019, 2020), previously presented by the authors.

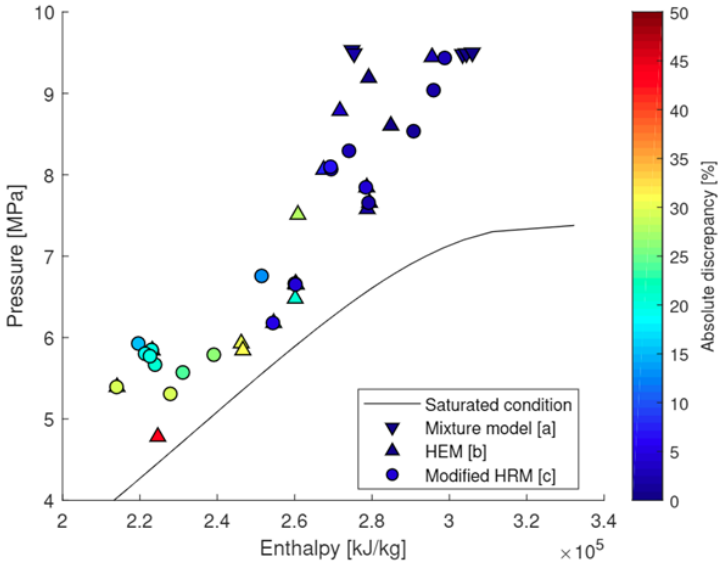

Figure 1: Summary of CFD model accuracy for motive nozzle mass flow rate (Ringstad et al., 2020)

2. MULTIPHASE MODELS

In this paper three multiphase models are presented, three pseudo-fluid models; (a) a homogeneous equilibrium model (HEM) based on the formulation by Smolka et al. (2013), (b) a mixture model based on the multi-species user-defined real-gas model (Giacomelli et al., 2019), (c) a homogeneous equilibrium model (HEM) based on the formulation by Haida et al., 2018, and (d) a two-fluid eulerian-eulerian model (Ringstad and Hafner, 2020). All models were implemented into ANSYS Fluent 19.2 through user defined functions, described in further detail below.

2.1. Homogeneous Equilibrium Model

Assuming equilibrium between the phases, i.e. equilibrium in pressure, velocity, temperature and chemical potential, a set of 2D transport equations for mass (Eq. 1), momentum (Eq. 2) and energy can be defined for a mixture of two phases. This model is referred to as the Homogeneous Equilibrium Model.

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho_m u_{mj}\right] = 0, \qquad \text{Eq. (1)}$$

$$\frac{\partial}{\partial t}(\rho_m u_{mi}) + \frac{\partial}{\partial x_j}\left[\rho u_{mi} u_{mj} + p_m \delta_{ij} - \tau_{mij}\right] = 0, \qquad \text{Eq. (2)}$$

Smolka et al. (2013) reformulated the energy equation into an enthalpy formulation in the form Eq. (3) which is introduced into ANSYS Fluent through a user-defined-scalar.

$$\nabla \cdot (\rho \vec{u} h) = \nabla \cdot (k_{\text{eff}} \nabla h) + \dot{S}_{h1} + \dot{S}_{h2} + \dot{S}_{h3}, \qquad \text{Eq. (3)}$$

Here, h is the specific enthalpy, $\vec{u}$ is the velocity vector, k_{eff} the effective diffusion coefficient, and the source terms $\dot{S}_{h1,2,3}$ describe the mechanical energy, the irreversible dissipation of the kinetic energy variations and the dissipation of the turbulent kinetic energy, respectively (Smolka et al., 2013). At homogeneous equilibrium, the enthalpy and pressure uniquely define a thermodynamic state in the two-phase dome:

$$\rho, \mu, k, \alpha, T, q = f(p, h), \qquad \text{Eq. (4)}$$

By assuming homogeneous equilibrium, the void-fraction is defined by the thermodynamic state as all phase change mechanisms are assumed to be instantaneous. A look-up table (100x100) was generated for the real fluid properties of R744 using the REFPROP (Lemmon et al., 2007) thermodynamic library calculated based on the Span-Wagner equation of state. The mixture viscosity and thermal conductivity based were found by a volume weighted average.

2.2. Homogeneous Relaxation Model

The mixture model is similar to the HEM based on the mixture averaged continuity, momentum and energy equations, Eqns. (1)- (3), also referred to as a pseudo-fluid approach. In the mixture model, thermodynamic non-equilibrium can be introduced by considering an additional equation for the transport of vapour fraction, Eqn. (5).

$$\frac{\partial}{\partial \mathrm{t}}(\rho_k \alpha_k) + \frac{\partial}{\partial \mathrm{x_j}}\left(\alpha_\mathrm{k}\rho_\mathrm{k}\mathrm{u_j}\right) = \Gamma, \qquad \text{Eq. (5)}$$

where Γ is a forcing term that describes the phase change mechanisms, and the offset from thermodynamic equilibrium. Previously, two formulations for the vapour fraction have been used for R744 ejector CFD models, the homogeneous relaxation models (Palacz et al., 2017, Haida et al., 2018), and the Mixture model (Giacomelli et al., 2019, Yazdani et al., 2012). The HRM treats the transition toward equilibrium as a relaxation process, governed by a relaxation time scale, θ, described in Eq. (6):

$$\Gamma_r = -\rho \frac{\beta - \beta_{eq}}{\theta} \qquad \text{Eq. (6)}$$

Here, β is the local flow quality and is the flow quality at equilibrium. The relaxation time has previously been studied by (Downar-Zapolski et al., 1996, Angielczyk et al, 2010, Haida et al., 2018). A relation for the relaxation time scale was found:

$$\theta = \theta_0 \alpha^a \phi^b \qquad \text{Eq. (7)}$$

Where, θ_0 is a scaling constant, α is the mixture void fraction, φ is a pressure parameters, and *a* and *b* are scaling parameters. The parameters *a* and *b* were investigated by Haida et al. (2018) and an optimized set was found, which is used in this work. The properties were defined as for the HEM, however the density was formulated using meta-stable liquid density from the REFPROP thermodynamic library, see the work by Palacz et al., 2017.

2.3. Mixure Model

Alternatively, the mixture model introduces non-equilibrium effects by directly modelling the phase change mechanisms between two phases. This is done by modelling the evaporation and condensation of the fluid with two terms, $\Gamma = \Gamma_c + \Gamma_e$. In this work, the Lee model is used to model phase change, Eqns. (6) and (7), similarly to previous works with this model (Giacomelli et al., 2018, 2019).

$$\Gamma_e = \sigma_e \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}}, \qquad \text{Eq. (7)}$$

$$\Gamma_c = \sigma_c \alpha_v \rho_v \frac{T - T_{sat}}{T_{sat}}, \qquad \text{Eq. (8)}$$

Numerical investigations of the R744 ejector using the mixture model (Giacomelli et al., 2018) found the evaporation and condensation constants that best fit experimental results were σ_e=100000 and σ_c= 0.1. These values were used for these simulations.

The two-phase mixture properties are defined by a mass or volume-based averaging of the two compressible phases. The phases are both evaluated by pressure and temperature, interpolated from a look-up table (152x126) based on the REFPROP thermodynamic library. The properties allow for meta-stable conditions of both liquid and

gas phase. The RERPROP library for R744 is based on the Span-Wagner equation of state, which is considered the most accurate EoS for CO_2 and is widely used for R744 ejector simulations.

2.4. Two fluid model

A two-fluid model solves one set of transport equation for each phase, *q*, with surrounding phases, *p*, Eqns. (8-10). The pressure, P_m is assumed equal for both phases.

$$\frac{\partial}{\partial t}(\alpha_q \rho_q) + \frac{\partial}{\partial x_j}\left[\alpha_q \rho_q u_{qj}\right] = 0, \qquad \text{Eq. (9)}$$

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q u_{qi}\right) + \frac{\partial}{\partial x_j}\left[\alpha_q \rho_q u_{qi} u_{qj} - \tau_{qij}\right] + R_{pq,i} + \left(\dot{m}_{pq} v_{pq,i} - \dot{m}_{qp} v_{qp,i}\right)$$

$$+\alpha_q \frac{\partial P_m}{\partial x_j}\delta_{ij} - F_{dispersed,i} = 0, \qquad \text{Eq. (10)}$$

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q h_q\right) + \frac{\partial}{\partial x_j}\left[\rho_q u_{qj} h_q + q_{qj} - u_{qi} T_{qij}\right] + Q_{pq} + h_{pq}\left(\dot{m}_{pq} - \dot{m}_{qp}\right) + \alpha_q \frac{\partial p_m}{\partial t} = 0, \qquad \text{Eq. (11)}$$

To successfully implement this model into ANSYS Fluent, some limitations of the software had to be overcome using *user-defined functions* (UDFs). Firstly, Fluent only allows for relations for specific heat as a function of temperature, $c_p = f(T)$. This was overcome by calculating a separate temperature field for the superheat of the liquid that includes superheat beyond the saturation temperature. Secondly, the interphasial enthalpy (the latent heat), h_{qp} must be defined as a single constant, here referred to as h_F. This issue was solved by introducing an additional source term to the liquid and gas energy-equations using a variable latent heat function and setting h_F to zero. For more details, see Ringstad and Hafner (2020).

The model includes several closure models, which allow adaptability and more advanced phase-coupling mechanisms than the simple pseudo fluid model. In this model the following closure models are used:

(a) Phase change: Lee model, see Eq. 7. and 8.

(b) Equation of state: Span-Wagner with non-equilibrium states, see Section 2.2.

(c) Momentum interaction: Schiller Neumann, see (ANSYS Fluent theory guide, 2019).

3. NUMERICAL MODEL SETUP

A numerical model was set up such that it could be compared to the experimental work by Palacz et al., 2017. The ejector geometry is described in Table 1.

Table1. Ejector dimensions

Dimension	EJ-2 (Palacz et al., 2017)
Inlet diameter, mm	3.80
Throat diameter, mm	1.41
Outlet diameter, mm	1.58
Converging angle	30.0°
Diverging angle	2.0°

A mesh convergence study was conducted with three 2D meshes, A, B, and C, with 6k, 25k and 100k cells, respectively. The ANSYS ICEM meshing software was used to generate structured meshes with high orthogonality

and low skewness, as in the previous work (Ringstad and Hafner, 2020). The mesh study indicated that mesh B was of high enough quality to properly describe the flow physics. For this study 3D effects are neglected due to computational limitations.

Four experimental cases presented by Palacz et al., 2017 are simulated. The experimentally messured conditions in these experiments are presented in Table 2. These values were used to calculate the boundary conditions of the simulations. A set of four points were chosen to get a selection of super critical, critical, and sub-critical operating conditions.

Table 2. Experimental conditions for R744 ejector operation (Palacz et al., 2017).

	P_{motive} [bar]	T_{motive} [C]	$P_{suction}$ [bar]	$T_{suction}$ [C]	P_{out} [bar]
1	53.93	6.33	27.3	5.7	34.23
9	66.51	22.41	28.21	2.21	34.85
14	75.79	28.07	28.17	2.58	36.80
18	94.46	35.28	27.21	2.60	32.85

The pressure-based implicit formulation in ANSYS Fluent was used in the calculations. This is the only option that is compatible with multiphase models in ANSYS Fluent. While it is generally agreed that density-based formulations performed better for highly compressible flows, pressure-based solvers have successfully been used for super sonic flows. The PRESTO! scheme was used for pressure and the second order upwind scheme was used for all other variables in the computations. The calculations with the HEM and HRM were done using a steady solver, which is a common assumption for R744 ejector flows. The mixture- and Eulerian model were run until steady state with a transient solver, to improve solver stability.

4. RESULTS AND DISCUSSION

4.1. Convergence

The simulations were run on 8 cores at 3.0 GHz clock frequency. The convergence criterion was based on steady residuals for all flow variables, as well as a steady solution for mass flow rates.

The HEM showed, in most cases, good stability and quite fast convergence, only somewhat dependent on initial and boundary conditions. The average case with 25k mesh-size would take approximately 70k iterations within 30-120 minutes. Some cases would not converge fully to the previously specified convergence criterion. This is likely due to the assumption of equilibrium not being fulfilled for those cases.

The HRM, similarly to the HEM shows good stability as long as appropriate formulations for the meta-stable density is used. It was found that using best fit functions for the data points provided better convergence and stability than using look-up table interpolation. The HRM would not converge as well for very low pressure conditions (Case #1). For this region it is suggested to converge, by first running with an HEM model or to use the mixture model presented by Bodys et al (2020). %. The HRM had some convergence issues, especially with second–order schemes. This may be due to numerical stiffness or implementation errors. When second-order schemes were applied to the vapour fraction transport equation became unstable.

The mixture model by Giacomelli (2019) showed very slow convergence rates and unstable behaviour, as previously reported by (Giacomelli et al., 2018, 2019). Depending on initial and boundary conditions, the simulations did not indicate convergence after 10 million iterations for the tested cases. The simulations indicated oscillating and diverging outlet flow rates, which would not satisfy mass conservation. The simulations were therefore stopped, as running until convergence could take up to several hundreds or thusands of CPU hours (Giacomelli et al., 2019). As the simulations did not converge, the simulations results are not used in further comparison.

The two-fluid model showed quite good convergence rates and would in most cases converge to a steady solution within 20-100k iterations, depending on the time-step size. The model showed stable convergence when appropriate initial conditions and phase change coefficients were chosen. However, finding these initial conditions was in certain cases challenging. Still, the model was found to be more stable than expected based on model complexity.

4.2. Comparison with previous results

The results of the simulations as well as the experimentally obtained values from Palacz et al (2015) are presented in Table 5.

Table 5: Comparison of numerical and experimental results;
The notation * indicates no suction flow, - indicates unstable simulation, ** indicates oscillating flow
TFM results from Ringstad and Hafner (2020).

	Experimental (kg/s)		HEM (%)		HRM (%)		TFM (%)	
case	m_m	m_s	Err_m	Err_s	Err_m	Err_s	Err_m	Err_s
1	0.099	0.0297	26.8	-3.0	-	-	-15.1	*
9	0.072	0.0137	17.5	-7.4	-9.8	-38.0	-8.5	-38.3
14	0.089	0.0249	28.2	42.6	-19.1	**	-13.6	-9.6
18	0.084	0.0353	0.3	1.1	-	-	13.6	-47.3

HEM shows that for decreaseing motive pressure the model accuracy drops. Additional test was conducted for the HEM at operating conditions near case 14, where much better accuracy was found, ie. motive MFR errors smaller than 7%. The results using the TFM results found in previous numerical results Ringstad and Hafner (2020). The accuracy is much below the HEM accuracy. Further work is suggested on this model to improve model accuracy.

5. CONCLUSION

All the discussed models (HEM, UDRGM Mixture, HRM, TFM) have previously shown to be able to predict R744 ejector flow with reasonable accuracy. In this work, it was found that the UDRGM mixture model is highly sensitive to initial conditions, is relatively unstable and has a high computational cost. This characteristic makes the UDRGM mixture model unreliable as a tool for optimization and rapid design. In comparison, the HEM, HRM and TFM can produce converged results within much shorter simulation time. Still, the more accurate thermodynamic library of the UDRGM shows in general a higher accuracy than other model in previous works. This motives research into efficiently implementing such a library in other models, such as the TFM.

The simulation results for the HEM are similar to those conducted in previous works, showing that the HEM can produce reasonable accuracy for super-critical operating conditions, but suffer at lower operating pressures. This implementation of the HRM showed poor convergence properties and would in general perform poorer than the HEM. However, previous versions of the HEM (Haida et al., 2018) have shown good convergence properties.The mixture model has been shown in previous studies to have very good accuracy (Giacomelli et al. 2019), however it was in this study found that the convergence rate of the model is too high for practical simulation. In comparison, the TFM produced results with lower accuracy, especially in the super-critical case. However, the TFM produced better results for lower operating conditions. The TFM can also be further improved by tuning the phase change parameters. The ability to add additional closure models to the TFM is its benefit as more physics can be incorporated into the simulations. This will bring the physical realism and model accuracy up with more research. Improving these submodels will however require extensive research into different flow phenomenons such as non-equilibrium thermodynamics, phase change modelling, two phase turbulence, and bubble break-up and coalescence, which is suggested as further work.

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NOMENCLATURE

cp	Specific Heat (kJ/kg)	q	Heat transfer (kW)	Γ	Phase change term (kg/s)
h	Specific enthalpy (kJ/kg)	R	Momentum interaction term (N/s)	μ	Viscosity (m^2/s)
k	Thermal conductivity (kW/K)	*T*	temperature (K)	ρ	Density (kg/m^3)
m	Mass transfer (kg/s)	*u*	Velocity (m/s)	σ	Phase change coeficiente (-)
P	pressure (Pa)	*α*	Volume fraction (m^3/m^3)	τ	Stress tensor (N/m^2)

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