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TWO-FLUID CFD MODEL FOR R744 TWO-PHASE EJECTORS

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ABSTRACT

This paper presents early results from a novel two-fluid Eulerian-Eulerian multiphase model for R744 two-phase ejectors, which to the authors knowledge has not previously been presented in literature. As opposed to previous R744 ejector models, this formulation includes non-equilibrium states for temperature, momentum, and chemical potential. The model is implemented into ANSYS Fluent using user-defined-functions and is able to achieve converged results faster than previous non-equilibrium formulations. Results are compared with experimental results. The mesh and model parameters are studied for their impact on accuracy.

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

1. INTRODUCTION

The current global warming crisis will require a large-scale response, calling for significant technological shifts in industries, worldwide. Responding to this, modern HVAC system are moving away from high global warming potential gases (GWP) refrigerants, such as the hydroflourocarbon (HFCs) gases. Instead, developing refrigeration technologies based on natural environmentally friendly refrigerants has been an important focus point of current research. Of the natural refrigerants, R744 (CO_2) has stood out due to its favourable thermo-physical properties (Kim et al. 2004), negligible GWP, non-flammability, non-toxicity and low cost. A critical enabling technology for R744 refrigeration systems is the two-phase ejector. A two-phase R744 ejectors is a work recovery device that allows for efficient R744 refrigeration, even in warm climates. However, improper design and control of two-phase ejectors can be detrimental for the system efficiency. Consequentially, much research has been devoted to developing advanced flow models for R744 ejector flow.

The model that has seen most use is the Homogeneous Equilibrium Model (HEM) (Smolka et al., 2013, Palacz et al., 2015). However, this model assumes full equilibrium between the phases. Palacz suggested that this model has a limited range of applicability and has significant errors at low pressure motive conditions that are often observed in R744 ejector system operation. Palacz suggested that at these low-pressure working conditions non-equilibrium effects are non-negligible, inciting research into non-equilibrium models. To account for these effects, a homogeneous relaxation model was presented (Palacz et al., 2017). Still, the HRM experiences significant errors at sub-critical motive pressures. An alternative approach was suggested by Giacomelli et al. (2018, 2019), where a mixture model was used to model a converging diverging nozzle (Giacomelli et al., 2018), and a R744 ejector (Giacomelli et al., 2019). The results showed good results for predicting the motive mass flow rate, however the computational cost of this model was found to be very high. In general, all models are still not able to accurately and reliably predict the suction nozzle mass flow rate accurately. This is likely because of the complexity of the driving mechanisms of the suction flow. To model these effects more advanced modelling tools are necessary. A model framework which enables more accurate modelling of these effects are the two-fluid models. These models are more complex as they involve a much larger set of coupling equations and more equations. For more details on R744 ejector models, see the detailed review of the state of the art R744 ejector models (Ringstad et al., 2019), previously presented by the authors.

2. MULTIPHASE MODELS

Multiphase models can be classified according to the number of equations solved. In general, the models are classified into two groups, pseudo-fluid models and two-fluid models (Eulerian-Eulerian). The pseudo-fluid models use an averaged set of equations for the mixture of the two phases. This reduces the number of equations to one set of transport equations, however, is based on several simplifying assumptions. On the other hand, two-fluid models use one set of equations for each phase. This model is therefore more physically realistic, however is dependent on several closure models. These closure models must be better understood to fully utilize the potential benefits of such a two-fluid model. In this paper a novel two-fluid eulerian-eulerian model for R744 ejectors is presented. To the authors knowledge this is the first full two-fluid model for R744 ejectors presented in the available literature. The model was implemented into ANSYS Fluent 19.2 through user defined functions, described in further detail below.

2.1. Two fluid model

The two-fluid model solves one set of transport equation for each phase, *q*, with surrounding phases, *p*, Eqns. (1-4). The pressure, P_m is assumed equal for both phases.

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

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q u_{qi}\right) + \frac{\partial}{\partial x_j}\left[\alpha_q \rho_q u_{qi} u_{qj} - T_{qij}\right] + R_{pq,i} + \left(\dot{m}_{pq} v_{pq,i} - \dot{m}_{qp} v_{qp,i}\right) + \alpha_q \frac{\partial P_m}{\partial x_j}\delta_{ij} - F_{dispersed,i} = 0, \qquad \text{Eq. (2)}$$

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q h_q\right) + \frac{\partial}{\partial x_j}\left[\rho_q u_{qj} h_q + q_{qj} - u_{qi} T_{qij}\right] + Q_{pq} + h_{pq}\left(\dot{m}_{pq} - \dot{m}_{qp}\right) + \alpha_q \frac{\partial p_m}{\partial t} = 0, \qquad \text{Eq. (3)}$$

$$\frac{\partial}{\partial t}(\alpha_q) + \frac{\partial}{\partial x_j}\left[\alpha_q u_{qj}\right] = 0, \qquad \text{Eq. (4)}$$

In these equations Einstein summation notation has been used for the directions with subscripts *i* and *j*. ρ, *u*, *h*, α are, respectively, the density, velocity, enthalpy, and phase volume fraction of the liquid or gas. The phase strain tensor is defined as $T_{qij} = \alpha_q \mu'_q (\frac{\delta u_i}{\delta x_j} + \frac{\delta u_j}{\delta x_i})$, where the phase viscosity is includes the contribution from turbulence. The heat flux in each phase, *q*, and interphasial heat transfer Q_{pq}, need special treatment, discussed below. Several phase interaction terms are included in this model. $R_{pq,i}$ is the momentum interaction term. Phase change models for the interphasial mass transfer, $\dot{m}_{pq}$ is discussed in below. Phase change will also introduce additional transfer of energy, H_{pq} and momentum, V_{pq}, which are the latent heat and drift velocity.

In this work, the Lee model is used to model phase change, Eqns. (5) and (6), similarly to previous works with this model (Giacomelli et al., 2018, 2019).

$$\dot{m}_{pq} = \sigma_e \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}}, \qquad \text{Eq. (5)}$$

$$\dot{m}_{qp} = \sigma_c \alpha_v \rho_v \frac{T - T_{sat}}{T_{sat}}, \qquad \text{Eq. (6)}$$

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. A study on the effects of these two coefficients in presented in this work.

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. The thermodynamic look-up tables are based on the work by Giacomelli et al., (2018), however only considers density, viscosity and speed of sound.

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, $c_p = f(T)$. Secondly, the interphasial enthalpy (the latent heat), h_{qp} must be defined as a single constant, here referred to as h_F. To correct for the issue of specific heat, a separate temperature field, T', is calculated using UDFs. The temperature field is calculated using a REFPROP look-up table in the liquid and gas regions up to the saturation point, such that $T'=f(P, h)$. Beyond the saturation point the non-equilibrium temperature is estimated by:

$$T'_{\text{superheated}} = T_{\text{saturated}} + \frac{h - h_{\text{sat}}}{c_p} \qquad \text{Eq. (7)}$$

Thus, the temperature field is independent of the specific heat defined in Fluent. To address the second issue, an additional source term, S_{pq}, is added to the enthalpy equation, Eq. (8), such that it would compensate for the constant value used in Fluent, with a latent heat that is a function of pressure, $h_{qp}(P)$.

$$\dot{S}_{pq} = \left[\dot{m}_{pq} - \dot{m}_{qp}\right]\left(h_{pq}(P) - h_{\text{F}}\right) \qquad \text{Eq. (8)}$$

Due to the change of temperature field, the interphasial heat transport models are not valid. Therefore, the inter-phasial heat exchange is assumed to be zero, $Q_{\text{pq}} = 0$. Furthermore, heat conduction is assumed negligible. These limitations are planned to be adressed in further work.

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

(b) Turbulence model for turbulent viscosity: Mixture formulation of k-epsilon realizable model

(c) Dispersion forces are neglected in this study.

Further testing and study of these closure models is necessary, however is left for future work.

3. NUMERICAL MODEL SETUP

The simulations were made to best reproduce the experimental results presented by (Palacz et al., 2017). Several 2D axi-symmetric structured meshes with N=6k, 25k and 100k cells were generated using the ANSYS ICEM meshing framework. The generated meshes were of high orthogonal quality with low skewness. The meshes were generated based on the dimensions used in the experimental and numerical investigations of Palacz et al., 2015. The boundary conditions for pressures and temperatures used are presented in Table 1, corresponding to the experimental conditions presented by Palacz et al. (2017). A set of four points were chosen to get a selection of super critical, critical, and sub-critical operating conditions due to the computational time constraint.

Table 1. 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 TFM model was run until steady state with a transient solver, to improve solver stability. The ejector simulations were performed with three different meshes, A, B, C, with 6k, 25k, and 100k cells, respectively. Table 2 shows the suction and motive massflow rates calculated using the different mesh resolutions for case 18.

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

	Case	mfr (kg/s)	Mesh		
			A	B	C
TFM (σ_e =5.0E+5)	18	M_m	0.0954	0.0954*	0.0961*
		M_s	0.0186	0.0207	0.0107

The two-fluid model achieves similar results for all meshes in terms of motive mass flow rate. However, mesh refinement introduces some oscillations to the motive flow. This was found to be caused by oscillations in the nozzle pressure-field. These oscillations might be caused by numerical errors or might be a physical phenomenon. The suction mass flow rate does not seem to be converged for this case. Prediction of the suction mass flow rate is in general very sensitive to the flow in the ejector. Due to the oscillations for finer meshes and faster computation time, mesh A was chosen for the TFM. However, it is expected that this will lower the TFM accuracy. The oscillating behaviors is believed to be caused by the thermodynamic properties and will be studied in further work.

4. RESULTS AND DISCUSSION

The phase change parameters are highly significant for the motive nozzle flow solution and the predicted mass flow rate. Therefore, a study on the evaporation coefficient σ_e was conducted to find the most appropriate coefficient with the Lee model. The results are shown in Table 3.

Table 3. Comparison motive mass flow rate with different evaporation phase change coefficient, Sigma e. Bolded text indicates solution used for comparison with experiments. (a) Oscillating outlet flow (b) Overheated gas (c) Unrealistic shock solution

M_m (kg/s)		Sigma e			
	Experiment	1E4	1E5	5E5	1E6
1	0.099	0.0850 (b)	**0.0841**	0.081 (a)	0.080 (a)
9	0.072	0.0851 (b)	**0.0659**	0.063 (a)	0.060 (a)

14	0.089	0.0954 (b)	**0.769**	0.068	0.067 (a)
18	0.084	0.112 (c)	0.102	**0.095**	0.094 (a)

The trend indicates that as σ_e is increased the motive mass flow rate is decreased, which is also seen in previous work (Palacz et al., 2017), where the HRM gives lower predicted mass flow rates than the HEM. Increase in σ_e is equivalent to bringing the thermodynamic state faster to equilibrium. Thus, it is expected that for super-critical flashing (case 18) the coefficient should be very high. Indeed, the trend indicates that even further increase in σ_e would be nessecary to achieve the experimentally observed motive mass flow rate. However, as σ_e was increased beyond 1.0E+5, the outlet mass flow rate would give oscillating results, noted in Table 3 with (a). This is believed to be caused by an oscillating mass transfer between the phases driven by the high coefficient. For low-pressure motive conditions (case 1) the simulations suggest that a lower mass transfer coefficient than 1E4 should be implemented. However, for very low values of σ_e, the delayed phase change will transfer too much energy into the gaseous phase, giving unrealistically high overheating of the gas beyond saturation. In total, these results motivate investigation into a more physically realistic mass-transfer model, which is left for further work.

Table 4: Comparison of numerical and experimental results; TFM with best coefficient from Table 4. The notation * indicates no suction flow.

	Experimental (kg/s)		TFM (%)	
case	m_m	m_s	Err_m	Err_s
1	0.099	0.0297	-15.1	*
9	0.072	0.0137	-8.5	-38.3
14	0.089	0.0249	-13.6	-9.6
18	0.084	0.0353	13.6	-47.3

The resulting mass flow rates with the TFM (with best match σ_e found in Table 3) are presented in Table 4. The TFM performed poorer than the HEM (Palacz et al., 2017). However, the TFM results were produced with a lower resolution mesh and without tuning for optimal coefficients. The TFM does however keep motive mass flow rate accuracy within 15% for all operating conditions, which can be improved by further tuning of the phase change coefficients. The suction mass flow rate is not well predicted by the TFM. This is expected as no emphasis has been put on turbulence or momentum interaction modeling in this work. Accounting for these effects is left for further work. Extensive research into appropriate closure models for this problem is nessecary to achieve realistic suction mass flow rate predictions. However, the potential to improve this prediction using advanced closure models is also the benefit of the TFM.

5. CONCLUSION

A novel two-fluid model (TFM) that accounts for thermal, velocity and thermodynamic non-equilibrium is presented in this work. A work-around that enables non-constant latent heat and pressure dependent specific heat in ANSYS Fluent is presented. The effects of phase change coefficients on model mass flow rate prediction is found to be significant. Still, further research is nessecary to improve model accuracy. The TFM produced results with lower accuracy than previous models. However, the TFM can also be further improved by tuning the phase change parameters. The ability to add additional closure models to the TFM is a benefit as more physics can be incorporated into the simulations. This will bring the models physical realism and 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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