

Advanced Numerical and Thermodynamic Modeling of CO₂ Ejectors for their Integration in Refrigeration Systems

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Contents

1	Introduction	1
1.1	Context	1
1.2	Fundamentals and advances in ejector technology	3
1.2.1	<i>Ejector basics</i>	3
1.2.2	<i>Ejector thermodynamic modeling</i>	6
1.2.3	<i>Modeling of CO₂ ejector refrigeration systems</i>	8
1.2.4	<i>Computational fluid dynamics of ejector flows</i>	10
1.2.5	<i>The challenges of experimental validation</i>	14
1.3	Positioning of the research work and objectives	15
1.4	Structure of the manuscript	17
2	A HRM in density-based formulation	19
2.1	Foreword	19
2.2	Introduction	20
2.3	Numerical methodology	25
2.3.1	<i>Geometrical modeling and operating conditions</i>	25
2.3.2	<i>Numerical modeling</i>	26
2.3.3	<i>Multiphase modeling</i>	27
2.3.4	<i>Tabulated method</i>	30
2.3.5	<i>Initial and boundary conditions and numerical procedure</i>	36
2.3.6	<i>Mesh grid</i>	37
2.4	Results and discussion	38
2.4.1	<i>Tabulated thermodynamic relations</i>	38
2.4.2	<i>Table speed-up</i>	41
2.4.3	<i>Validation and verification of the solver</i>	42
2.4.4	<i>Homogeneous equilibrium vs homogeneous relaxation</i>	44
2.5	Conclusions	49

3	Performance analysis of the ERS	51
3.1	Foreword	51
3.2	Introduction	52
3.3	Thermodynamic modeling	55
3.3.1	<i>Cycle modeling</i>	55
3.3.2	<i>Ejector thermodynamic model</i>	59
3.4	Results and discussion	61
3.4.1	<i>Entrainment ratio maps</i>	62
3.4.2	<i>Operation of the ERS</i>	63
3.4.3	<i>Influence of the geometry on the COP</i>	66
3.4.4	<i>Analysis of the ejector regime</i>	70
3.4.5	<i>High temperature gas cooler</i>	72
3.5	Conclusions	73
4	Optimal ejector exergy efficiency and COP	75
4.1	Foreword	75
4.2	Introduction	76
4.3	Numerical methodology	81
4.3.1	<i>General procedure</i>	81
4.3.2	<i>Geometrical modeling and operating conditions</i>	82
4.3.3	<i>CFD modeling and validation</i>	83
4.3.4	<i>Exergy tube method</i>	87
4.3.5	<i>Thermodynamic modeling</i>	89
4.4	Results and discussion for transcritical operations	91
4.4.1	<i>Operation curves</i>	91
4.4.2	<i>Exergy transfers vs COP</i>	94
4.5	Results and discussion for subcritical operations	97
4.5.1	<i>Operation and exergy transfers at equilibrium</i>	97
4.5.2	<i>Impact of metastability</i>	101
4.6	Conclusions	105
5	Conclusions	109
5.1	Specific achievements	110
5.1.1	<i>Modification and implementation of CFD tools</i>	110
5.1.2	<i>ERS thermodynamic modeling</i>	111
5.1.3	<i>Multi-scale analysis of the ejector within the ERS</i>	112
5.2	Research perspectives	113
A	List of Publications	117

B	Complementary Analyses	121
2.1	Exergy gains required by the cycle	121
2.2	COP improvement compared to the basic four-components cycle	125
C	An improved ejector thermodynamic model	129
3.1	Introduction	129
3.2	Ejector model and solving algorithm	133
3.2.1	<i>Assumptions</i>	133
3.2.2	<i>Modeling of on-design operation using the compound-choking criterion</i>	134
3.2.3	<i>Modeling of off-design operation</i>	138
3.3	Validation of the thermodynamic model for single-phase ejectors	144
3.3.1	<i>Relation between Fabri-choking and compound-choking</i>	144
3.3.2	<i>Influence of the isentropic efficiencies on the characteristic curves</i>	146
3.3.3	<i>Fitting to R134a ejector experimental data</i>	149
3.3.4	<i>Fitting to air ejector experimental data</i>	151
3.4	Relation between the compound-choking criterion and the maximization of the mass flow rate	152
3.4.1	<i>Non-isentropic nozzle flow of a perfect gas</i>	152
3.4.2	<i>Compound-choking criterion</i>	155
3.4.3	<i>Mass flow rate maximization for a supersonic ejector</i>	157
3.5	Conclusion	159
D	Investigation of a CO₂ heat pump using dymola	161
4.1	Introduction	161
4.2	Limitations of TIL ejector models	162
4.3	Ejector model implementation in dymola	164
4.4	Calibration for CO ₂ heat pump applications	166
4.5	Investigation on ejector size	167
4.6	Conclusions	169
	Bibliography	171

List of Figures

1.1	Comparison of the transcritical CO ₂ refrigeration cycle to conventional refrigerants cycles at an evaporator temperature of 15 [°C] and gas cooler/condenser temperature of 35 [°C] (reproduced after [52]). The pressure drop at the expansion valve, Δp , is of $\Delta p = 3.98$ [bar] with R134a, $\Delta p = 8.89$ [bar] with R410a, and $\Delta p = 48.63$ [bar] with CO ₂	3
1.2	Schematics of a typical ejector [53].	4
1.3	Typical characteristic curve of an ejector.	5
1.4	Layout of a typical ejector with discrete sections (labeled from 0 to d) used in a thermodynamic model.	6
1.5	Layout of a typical CO ₂ ejector refrigeration system.	9
2.1	Two-dimensional mesh for the nozzle c of [117] with relevant notations. The related dimensions for the different geometries are given in Table 2.1.	26
2.2	Flowchart of the HRM algorithm in density-based formulation. .	30
2.3	Range of operation (in blue) of the nozzle of Nakagawa et al. [117] (case c , see Tab. 2.1). The saturation dome is highlighted in red with the critical point marked with the black dot. The dashed curve is the isentropic expansion, for reference.	32
2.4	Schematic of an individual cell taken in the state-space domain. The thermodynamic relation is interpolated on 16 equally-spaced points and the error is calculated at 9 locations called verification points.	33
2.5	Flowchart of the grid generation algorithm for the look-up table.	35
2.6	Properties in the $p - e$ state space and mesh generated by the tabulation algorithm. The imposed precision for the tables is 0.1 [Pa] for pressure and 0.0001 [K] for temperature.	39

★ | List of Figures

2.7	Relatives errors in the $\rho - e$ state space.	40
2.8	Density in the $\rho - e$ state space including the metastable region. In Figure 2.8a, the invalid states are represented in gray, and the saturation curve (plain curve) and the approximated spinodal limit (dashed curve) are plotted.	40
2.9	Performance comparison between the present tabulated method and the one of [56].	41
2.10	Pressure profiles along the center-line of the nozzle (CFD) and comparison with the experimental data of Nakagawa et al. [117]. Please refer to Table 2.1 for geometrical and inlet parameters of cases a, b and c.	43
2.11	Pressure profiles obtained for case c using HEM and HRM with different constant relaxation times and the correlation of [7], and comparison with experimental measurements [117].	45
2.12	Relative difference of quality with respect to the equilibrium and pressure profiles using different methods at the center line and at the wall for case c.	46
2.13	Quality profiles obtained for case c using HEM and HRM with different constant relaxation times and the correlation of [7]. . .	47
2.14	Fields of the mean axial velocity component obtained for case c using HEM and HRM with different relaxation times. The geometry was stretched X4 in the vertical direction for better readability.	48
2.15	Density fields obtained for case c using HEM and HRM with different relaxation times. The geometry was stretched X4 in the vertical direction for better readability.	48
3.1	Classical ejector refrigeration system. The main locations of the cycle have been numbered for reference within the text.	56
3.2	Classical ERS represented in the $p - h$ diagram. Operating conditions are $p_{gc} = 100$ [bar], $p_{out} = 35$ [bar], $T_{amb} = 25$ [°C] and $T_{cool} = 4$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). Note that the y axis is in log scale.	58
3.3	Schematic of the ejector model, after Metsue et al. [110].	59

3.4	Fitting of the ejector model onto the experimental data of Zhu et al. [155] ($\eta_p = 0.95$, $\eta_{py} = 0.73$, $\eta_s = 0.73$, $\eta_m = 1$, $\eta_d = 0.85$). The experimental data are shown with squares and the thermodynamic model predictions in plain lines.	61
3.5	Maps of the entrainment ratio ω as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} for $T_{amb} = 25$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). Iso- ω lines are plotted in black.	62
3.6	Map of the COP as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} . The purple line is the operation curve with the fitting for the ejector of [155] and the green line the case with all $\eta_i = 1$. The on-/off-design limit is plotted in dotted lines and the maximum COPs are highlighted with dots.	64
3.7	Operation curves and characteristic curves for $T_{amb} = 25$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]) with different sets of efficiencies. Unless indicated otherwise in the legend, all efficiencies are set to unity. In Fig. 3.7a, the plain and dashed curves indicate on-design and off-design regime, respectively, and the dotted lines are iso-COPs.	65
3.8	Maps of the COP as a function of the gas cooler pressure and the TAR. The dot and star indicate the locations of the maximum COP with the original geometry of [155], and the global maximum COP, respectively.	67
3.9	Maps of the COP as a function of the gas cooler pressure and A_e/A_t for $T_{amb} = 25$ [°C], $T_{cool} = 4$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). The dot and star (Fig. 3.9a) indicate the locations of the maximum COP with the original geometry of [155], and the global maximum COP, respectively.	70
3.10	Maximum COP operation points (diamonds) on their characteristic curve for each optimal geometry and for various ambient temperatures. The case with all $\eta_i = 1$ is also shown for reference. The operation points correspond to those in Table 3.2.	71
3.11	Map of the COP as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} for $T_{amb} = 65$ [°C], $T_{cool} = 4$ [°C] ($T_3 = 75$ [°C], $T_{10} = -6$ [°C]). The purple line is the operation curve with the fitting for the ejector of [155]. The on-/off-design limit is plotted in dotted line and the maximum COP is highlighted with the dot.	72

★ | List of Figures

4.1	Classical ejector refrigeration system. The different points are numbered for reference in the text.	77
4.2	Flowchart of the procedure that is applied in the present work to determine if there is a correlation between optimal exergy transfers within the ejector and maximum COP of the cycle (red arrow).	81
4.3	Two-dimensional mesh of the ejector (axisymmetric view). By convention, the zero axial coordinate is set at the primary nozzle exit.	85
4.4	Pressure profiles at the centerline of the ejector obtained with the regular and finer meshes ($T_{gc} = 35$ [°C], $p_{gc} = 8.50$ [MPa], $p_{out} = 3.40$ [MPa]).	85
4.5	Two-dimensional schematic displaying the relevant surfaces/volumes for the exergy tube analysis (axisymmetric view). The dividing streamline is plotted in red. The gray area is $V_2(z)$ and the dashed line $S(z)$	88
4.6	Fitting of the characteristic curves (plain line) onto the CFD-HEM results (squares). The related fitting efficiencies are given in Table 4.4.	92
4.7	COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Discrete CFD calculation points are indicated by the squares (same colors as in Figure 4.6) and the maximum COPs along the operation curves are highlighted by stars. Iso-COP lines are plotted in black.	93
4.8	Dimensionless exergy gain and destruction along the axial direction of the ejector (Fig. 4.5) for $T_{gc} = 35$ [°C] and $p_{gc} = 8.5$ [MPa].	94
4.9	Dimensionless net exergy gain of the secondary stream for $T_{gc} = 35$ [°C] and $p_{gc} = 8.5$ [MPa].	95
4.10	Dimensionless net outlet exergy gains of the secondary stream Δ_{out} as a function of the compression ratio. The diamonds indicate the points of intersection with the operation curve. . .	96
4.11	Net outlet exergy gains of the secondary stream δ_{out} as a function of the compression ratio. The diamonds indicate the points of intersection with the operation curve.	97

4.12	Fitting of the characteristic curves (plain line) onto the CFD-HEM results (squares) for $T_{gc} = 25$ [°C]. The related fitting efficiencies are given in Table 4.5.	98
4.13	Map of the COP as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . The partial operation curve is plotted with green diamonds and dashed line. Discrete CFD calculation points are indicated by the squares and the maximum COP along the operation curve ($COP_{max} = 5.28$ at $p_{out}/p_{evap} = 1.078$) is highlighted by the star. Iso-COP lines are plotted in black.	99
4.14	Ejector refrigeration cycle in the $p - h$ diagram. In red: the saturation curve and critical point (dot); black line: iso-temperature $T_{gc} = 25$ [°C]. The cycle is represented for four p_{gc} values including the two limit states at the discontinuity. Point 3 is located on the iso-temperature by construction of the model.	100
4.15	Net outlet exergy gains of the secondary stream as a function of the compression ratio for $T_{gc} = 25$ [°C]. The diamonds indicate the point of intersection with the operation curve.	101
4.16	Primary/secondary mass flow rates and entrainment ratios using the HEM and HRM ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]). . .	102
4.17	Pressure and axial velocity contours obtained using the HEM (top half) and HRM with $\theta = 4.10^{-6}$ [s] (bottom half) (zoom on the relevant portion of the ejector). Results for $p_{gc} = 6.55$ [MPa], $T_{gc} = 25$ [°C] and $p_{out}/p_{evap} = 0.96$	102
4.18	Dimensionless exergy gain and destruction terms for $\theta = 4.10^{-6}$ [s] ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]).	103
4.19	Dimensionless net exergy gain of the secondary stream in HEM and HRM with $\theta = 4.10^{-6}$ [s] ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]).	104
4.20	Net outlet exergy gains of the secondary stream as a function of the compression ratio with the HEM and HRM ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]). The diamonds indicate the point of intersection with the operation curve.	105

★ | List of Figures

- B.1 COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP and iso- Δ_{out} are plotted in plain black and dotted black, respectively. The maximum COP (also maximum Δ_{out}) along the operation curve is highlighted by the star. 122
- B.2 COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP and iso- δ_{out} (in [W]) are plotted in plain black and dotted black, respectively. The maximum COP and maximum δ_{out} along the operation curve are highlighted by the black and blue stars, respectively. 122
- B.3 Dimensional (black) and dimensionless (blue) net exergy gains obtained from cycle requirements and values obtained at the ejector outlet. The stars indicate the maximum of the cycle requirements curves. Results are obtained for two gas cooler temperatures: (a) $T_{gc} = 35$ [°C] and (b) $T_{gc} = 36$ [°C]. 123
- B.4 Total specific exergy profile at the outlet of the ejector along the radial direction at two different operation points ($T_{gc} = 35$ [°C]). The radial coordinate is r and the diffuser outlet radius is r_{out} . . . 124
- B.5 COP maps as a function of the condenser pressure p_{cond} and the compression ratio p_{out}/p_{evap} at $T_{gc} = 25$ [°C]. The operation curve is plotted in green (diamonds and dashed line), iso-COPs are plotted in plain black, and iso- Δ_{out} and iso- δ_{out} are plotted in dashed and dotted black, respectively. The maximum COP and maximum δ_{out} along the operation curve are highlighted by the black and blue stars, respectively. 125
- B.6 Schematic of the classical 4-components refrigeration cycle. . . 126
- B.7 Maps of the COP improvement ratio of the ejector cycle compared to the classical cycle, as a function of p_{gc} or p_{cond} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP ratios are plotted in plain black. The maximum COP and maximum COP improvement along the operation curve are highlighted by the black and blue stars, respectively. 126

B.8	Maps of the COP improvement ratio of the ejector cycle compared to the classical cycle, as a function of the condenser pressure p_{cond} and the compression ratio p_{out}/p_{evap} . The operation curve is plotted in plain green (diamonds and dashed line). Iso-COP ratios are plotted in plain black. The maximum COP and maximum COP improvement along the operation curve (superimposed) are highlighted by the black star.	127
C.1	Typical characteristic curve of an ejector.	130
C.2	Schematic diagram of the ejector model (top half).	134
C.3	Variations of the mass flux G as a function of the primary flow pressure p_p for three stagnation temperatures. Results obtained for R134a with $p_{p,0} = 1.934$ [MPa] and $\eta_p = 0.97$	136
C.4	Flowchart of the model for on-design operations using the compound-choking criterion (Fig. C.2).	139
C.5	Flowchart of the model for off-design operation.	143
C.6	Comparison between Fabri-choking and compound-choking for $p_{p,0}/p_{s,0} = 4.5$. The working fluid is air and $\eta_m = 0.92$. The positions of the critical conditions have been highlighted on the ω -curve.	145
C.7	Influence of the different isentropic efficiencies on the characteristic curves using the compound-choking based model. The Fabri-choking model is also displayed for comparison purpose.	147
C.8	Characteristic curve obtained for the geometry of Garcia del Valle et al. [60].	149
C.9	Characteristic curves obtained for the ejectors of Hakkaki-Fard et al.	150
C.10	Characteristic curves obtained for the air ejector test bench of Université catholique de Louvain with $\eta_p = 0.977$, $\eta_s = 0.75$ and $\eta_m = 0.95$. Comparison between the present thermodynamic model and new experimental data.	152
C.11	Corrected characteristic curves obtained for the air ejector test bench at Université catholique de Louvain with $\eta_p = 0.977$, $\eta_s = 0.71$ and $\eta_m = 0.95$. Comparison between the present thermodynamic model and new experimental data.	158
D.1	Comparison of the two ejectors models in TIL with the present model.	163
D.2	Schematic of the ejector model of Metsue et al. [110].	164

★ | List of Figures

D.3	Fitting of the model onto the experimental data of Zhu et al. [155]. Blue: $p_{p,0} = 87$ [bar]; Red: $p_{p,0} = 93$ [bar]; Black: $p_{p,0} = 98$ [bar].	166
D.4	Schematic of the ejector-based heat pump cycle working with CO ₂ .	167
D.5	Ejector operating conditions and COP of the cycle as a function of the ejector size. The dashed line delimits on- and off-design regimes.	168

List of Tables

1.1	Environmental and health properties of current and potential future refrigerants, adapted from [45].	2
2.1	Dimensions and operating conditions of the nozzles considered by [117].	26
2.2	Mass flow rate and increase with respect to the HEM solution for case c with various relaxation times and the correlation of [8].	49
3.1	Pair of state variables to solve the cycle at each relevant point.	58
3.2	Maximum COP obtainable along the operation curve for the three studied T_{amb} values and for the base (Zhu et al. [155]) and optimal geometries (O.G.) obtained for those temperatures (Fig. 3.8). Efficiencies are calibrated on [155].	68
3.3	Gas cooler pressures, ejector mass flow rates and throat diameters for optimal operation (Fig. 3.8) at each ambient temperature. The ejector model is calibrated on Zhu et al. [155].	69
4.1	Dimensions of the ejector.	82
4.2	Operating conditions used for the CFD simulations. The ellipses (...) indicate intermediate values, equally spaced by 0.1 [MPa].	83
4.3	Predictions of the primary and secondary mass flow rates and comparison with the experimental data of [20].	86
4.4	Fitting efficiencies for each set of gas cooler exit temperature and pressure (Fig. 4.6).	92
4.5	Fitting efficiencies for each gas cooler exit pressure at $T_{gc} = 25$ [°C].	98

★ | List of Tables

C.1	Geometry and operating conditions for the three experiments of Hakkaki-Fard et <i>al.</i> [71].	151
D.1	Operating conditions.	163
D.2	Main parameters for the simulation of the cycle.	168

List of Symbols

Alphanumerics	Definition	Units
a	Speed of sound	$[\text{m.s}^{-1}]$
A	Area	$[\text{m}^2]$
AR	Aspect ratio	$[-]$
D	Diameter	$[\text{m}]$
D	Displacement	$[\text{m}^3]$
e	Specific internal energy	$[\text{J.kg}^{-1}]$
e_x	Streamwise direction	$[-]$
F_{ξ}	Exergy flux	$[\text{W.m}^{-2}]$
G	Mass flux	$[\text{kg.m}^{-2}.\text{s}^{-1}]$
h	Specific enthalpy	$[\text{J.kg}^{-1}]$
I_{ξ}	Dimensionless exergy gain	$[-]$
k	Turbulence kinetic energy	$[\text{J.kg}^{-1}]$
L	Ejector length	$[\text{m}]$
M	Mach number	$[-]$
$\dot{m}$	Mass flow rate	$[\text{kg.s}^{-1}]$
p	Pressure	$[\text{Pa}]$
q	Heat flux	$[\text{J.m}^{-2}.\text{s}^{-1}]$
$\dot{Q}$	Heat power	$[\text{W}]$
r	Radial coordinate	$[\text{m}]$
R	Specific gas constant	$[\text{J}.\text{(kg.K)}^{-1}]$
Re	Reynolds number	$[-]$
s	Specific entropy	$[\text{J}.\text{(kg.K)}^{-1}]$
S	Surface	$[\text{m}^2]$
T	Temperature	$[\text{K}]$
t	Time	$[\text{s}]$
u	Velocity	$[\text{m.s}^{-1}]$

★ | List of Symbols

Alphanumerics	Definition	Units
V	Velocity	$[\text{m.s}^{-1}]$
V	Volume	$[\text{m}^3]$
$\dot{V}$	Volume flow rate	$[\text{m}^3.\text{s}^{-1}]$
$\dot{W}$	Work power	$[\text{W}]$
x	Horizontal coordinate	$[\text{m}]$
x	Vapor quality	$[-]$
z	Axial coordinate	$[\text{m}]$
Greek Letters	Definition	Units
α	Void fraction	$[-]$
β	Compound flow indicator	$[m^2]$
δ	Net exergy gain	$[\text{W}]$
Δ	Dimensionless net exergy gain	$[-]$
γ	Heat capacity ratio	$[-]$
ϵ	Error tolerance	$[-]$
η	Efficiency	$[-]$
θ	Relaxation time	$[\text{s}]$
κ	Thermal conductivity	$[\text{W}.\text{(m.K)}^{-1}]$
ξ	Specific exergy	$[\text{J}.\text{kg}^{-1}]$
ρ	Density	$[\text{kg}.\text{m}^{-3}]$
τ	Stress tensor	$[\text{kg}.\text{m}^{-1}.\text{s}^{-2}]$
Φ	Exergy losses	$[\text{W}.\text{m}^3]$
Π	Dimensionless exergy losses	$[-]$
ω	Entrainment ratio	$[-]$
ω	Specific dissipation rate	$[\text{s}^{-1}]$
Subscripts	Definition	
0	Inlet/Stagnation conditions	
2	Diffuser inlet	
amb	Ambient	
c	Critical point	
c	Setpoint back pressure	
$cond$	Condenser	
$cool$	Cooling	
$comp$	Compressor	
$crit$	Critical point	
d	Diffuser outlet	
e	Primary nozzle exit	

Subscripts	Definition
<i>eq</i>	Equilibrium
<i>ev</i>	Evaporator
<i>evap</i>	Evaporator outlet
<i>gc</i>	Gas cooler
<i>guess</i>	Guessed value
<i>h</i>	Hydraulic
<i>in</i>	Inlet
<i>l</i>	Liquid phase
<i>m</i>	Mixed flow
<i>max</i>	Maximum
<i>ml</i>	Metastable liquid
<i>N</i>	Normal shock
<i>out</i>	Ejector outlet
<i>p</i>	Primary stream
<i>pol</i>	Polytropic
<i>ref</i>	Reference state
<i>s</i>	Secondary stream
<i>sat</i>	Saturated conditions
<i>sl</i>	Saturated liquid
<i>sv</i>	Saturated vapor
<i>t</i>	Throat
<i>t</i>	Total quantity
<i>v</i>	Vapor phase
<i>w</i>	Wall
<i>y</i>	Aerodynamic throat
Superscripts	Definition
<i>t</i>	Turbulent
*	Critical conditions

List of Abbreviations

Abbreviation	Definition
CFC	Chlorofluorocarbon
CFD	Computational Fluid Dynamics
CFL	Courant–Friedrichs–Lewy
CO ₂	Carbon Dioxide
COP	Coefficient of Performance
DEM	Delayed Equilibrium Model
DNS	Direct Numerical Simulation
EoS	Equation of State
ERS	Ejector Refrigeration System
FANS	Favre-Averaged Navier-Stokes
GWP	Global Warming Potential
HCFC	Hydrochlorofluorocarbon
HEM	Homogeneous Equilibrium Model
HFC	Hydrofluorocarbon
HRM	Homogeneous Relaxation Model
IIR	International Institute of Refrigeration
LES	Large Eddy Simulation
NXP	Nozzle Exit Position
ODP	Ozone Depletion Potential
PDE	Partial Differential Equation
PG	Perfect Gas
PR	Peng-Robinson
R744	Carbon Dioxide
RANS	Reynolds-Averaged Navier-Stokes
SG	Stiffened Gas

★ | List of Abbreviations

Abbreviation	Definition
SST	Shear-Stress Transport
SW	Span-Wagner
TAR	Throat Area Ratio
TKE	Turbulence Kinetic Energy

1

Introduction

1.1 Context

The global energy situation has become a major concern. While fossil energy sources become scarcer, the energy demand keeps increasing, and the environmental impact on climate becomes a growing preoccupation as climate change leads to a rapid increase in the energy needed for cooling purposes. According to the International Institute of Refrigeration (IIR), the total number of refrigeration, air-conditioning, and heat pump systems in operation worldwide was about 5 billions as of 2019 [47]. Any small improvement in the efficiency of such devices would, therefore, have a significant impact. In addition, the IIR estimated that around 20% of the global warming impact of refrigeration systems is due to direct emissions (leakage) of chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), and hydrochlorofluorocarbons (HCFCs) [47]. Consequently, European legislation imposed restrictions on the use of refrigerants with a high ozone depletion potential (ODP) and a global warming potential (GWP) greater than 150. Most synthetic refrigerants, such as R11, R22, R134a, R245fa, . . . , do not meet these restrictions. Likewise, Canada has decided, after the Montreal Protocol of 1987 and the Kigali Amendment of 2016, to reduce the production and consumption of HFCs by more than 80% by 2045 [144]. Instead, so-called natural refrigerants should be used, as they have little to

Fluid	Formula	Toxicity	Flammability	ODP	GWP
R-12	CCl_2F_2	Nontoxic	Nonflammable	1.0	10 900
R-114	$\text{C}_2\text{Cl}_2\text{F}_4$	Nontoxic	Nonflammable	1	10 000
Propane	C_3H_8	Low	Very high	0	3
i-Butane	$\text{i-C}_4\text{H}_{10}$	Low	Very high	0	3
n-Butane	C_4H_{10}	Low	Very high	0	3
i-Pentane	$\text{i-C}_5\text{H}_{10}$	Low	Very high	0	3
n-Pentane	C_5H_{12}	Low	Very high	0	3
R-32	CH_2F_2	Low	Low flammable	0	675
R-134a	$\text{C}_2\text{H}_2\text{F}_4$	Very low	Nonflammable	0	1 430
R-245fa	$\text{C}_3\text{H}_3\text{F}_5$	Very low	Nonflammable	0	1 020
Carbon dioxide	CO_2	Nontoxic	Nonflammable	0	1.0
Ammonia	NH_3	Toxic	Lower	0	0
Water	H_2O	Nontoxic	Nonflammable	0	–

Table 1.1 Environmental and health properties of current and potential future refrigerants, adapted from [45].

no impact on climate change [2].

Carbon dioxide (CO_2 , R744) is therefore an appropriate replacement for conventional refrigerants. Indeed, it is seen in Table 1.1 that CO_2 has a zero ODP and a GWP of 1, which is hundreds of times less harmful than classical refrigerants such as R134a. In addition, this refrigerant has the advantage of being non-toxic and non-flammable. However, typical CO_2 refrigeration cycles suffer from low performance compared to cycles using classical refrigerants [52]. Because of the thermodynamic properties of carbon dioxide, namely, a critical temperature of 31 [°C] which is relatively close to the ambient, CO_2 refrigeration cycles must often operate at high pressures to reach temperatures enabling heat transfers with the ambient. Practically, this implies that, depending on the ambient conditions, the cycle may frequently operate under transcritical operation, which characterizes a thermodynamic cycle in which the working fluid goes through both subcritical and supercritical states. Expansion losses are then substantial because of the high pressure difference [79]. To illustrate this, one can refer to Figure 1.1, which compares a classical refrigeration cycle working with R134a, R410a, or CO_2 whilst operating at the same temperatures. As visible in Figure 1.1, the expansion part in the CO_2 cycle also generates significantly more entropy, and hence related throttling losses, than with other

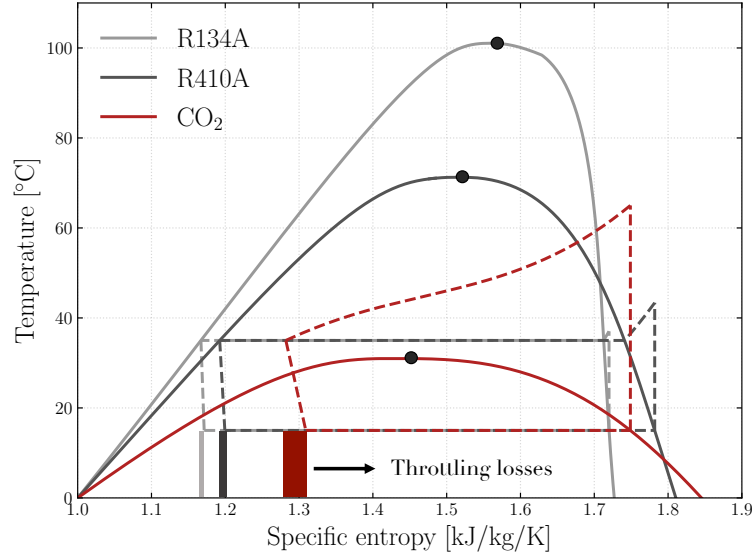


Fig. 1.1 Comparison of the transcritical CO₂ refrigeration cycle to conventional refrigerants cycles at an evaporator temperature of 15 [°C] and gas cooler/condenser temperature of 35 [°C] (reproduced after [52]). The pressure drop at the expansion valve, Δp , is of $\Delta p = 3.98$ [bar] with R134a, $\Delta p = 8.89$ [bar] with R410a, and $\Delta p = 48.63$ [bar] with CO₂.

classical refrigerants. In other words, the exergy losses (losses associated with entropy production) are greater, also leading to the fact that CO₂ has a higher potential for efficiency improvement (mechanical work recovery). To enhance the performance of refrigeration cycles and balance out the low performance of such systems when operating with natural refrigerants such as CO₂, one compelling strategy is to integrate an ejector within the cycle [17, 50, 66, 91]. Ejectors are favorable devices used to suck and compress fluids that find one of their main application in the field of refrigeration.

1.2 Fundamentals and advances in ejector technology

1.2.1 Ejector basics

As shown in Figure 1.2, ejectors are passive devices that can be broken down into four parts: the primary nozzle, the mixing chamber, the mixing duct (also referred to as the secondary throat), and the diffuser. Under standard operation of the device, a motive fluid at high stagnation pressure

1 | Introduction

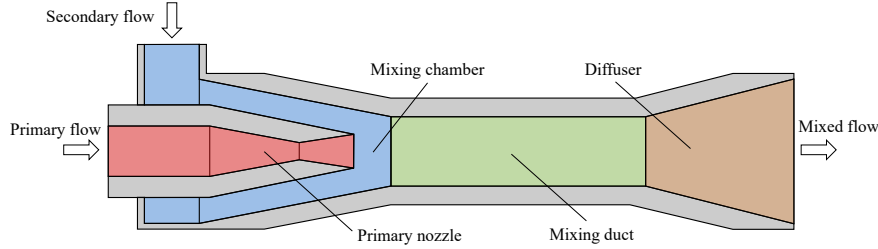


Fig. 1.2 Schematics of a typical ejector [53].

is expanded in a primary nozzle, converting its pressure energy into kinetic energy. In the case of a two-phase ejector, if the motive fluid enters the nozzle under liquid or supercritical conditions, a flashing phenomenon appears just after the primary nozzle throat as the fluid goes from the liquid state to a liquid/vapor mixture. This causes a sharp decrease in sound velocity, so that the flow becomes supersonic [26]. The two-phase low-pressure supersonic jet at the outlet of the primary nozzle draws and compresses a secondary fluid at low stagnation pressure by means of complex exergy exchanges through a compressible and turbulent shear layer along the ejector. Primary and secondary fluids mix in the mixing chamber and the mixing duct to end up with an intermediate stagnation pressure at the diffuser outlet. Complex shock wave and expansion fan patterns may occur within the primary nozzle, mixing chamber, mixing duct, and diffuser. The position and intensity of these phenomena depend on the geometry and operating conditions [106]. Additionally, metastable phenomena may occur depending on the primary inlet conditions [122], since in such highly compressible flows, the phase change significantly depends on the rate of bubble nucleation [124]. The expansion is so fast, inducing high velocities and a low residence time, that the fluid may not have sufficient time to reach equilibrium and vaporize under the usual saturation conditions. Consequently, there is a delay before the flow returns to the liquid-vapor equilibrium state. This practical implication results in distinct flow topologies, thermodynamic states, and higher mass flow rates than equilibrium conditions [40, 122].

Depending on the operating conditions, ejectors can work under different regimes that characterize both their performance in terms of mass flow rates and their internal flow topology. In supersonic ejectors, the primary flow is said to be *choked*, in the sense that the mass flow rate is independent

of downstream conditions [136]. Depending on the secondary inlet and ejector outlet operating conditions, the secondary stream may be choked as well [3]. To qualify the operating regime of the device and quantify its performance, characteristic curves are commonly employed, that are curves of the entrainment ratio $\omega = \dot{m}_s / \dot{m}_p$ (with $\dot{m}_s$ and $\dot{m}_p$ the secondary and primary mass flow rates, respectively) versus the pressure at the outlet of the device p_{out} . Figure 1.3 depicts a typical characteristic curve of an ejector. Much as for a simple nozzle, if the outlet pressure is below a critical pressure p_{out}^* , the entrainment ratio is maximum and independent of the outlet pressure. Both primary and secondary flows are choked, and the ejector is consequently said to be operating under the on-design (or double-choking) regime. If $p_{out} > p_{out}^*$, the entrainment ratio decreases as p_{out} increases, and the ejector is said to be operating under the off-design (or single-choking) regime. If $p_{out} = p_{out}^*$, the ejector is said to be operating under critical operating conditions, in which the highest outlet pressure with maximum entrainment ratio is obtained. Lastly, if the outlet pressure exceeds the so-called breakdown pressure, the ejector is malfunctioning, as part of the flow goes back into the secondary inlet.

Ejectors are known for their complex fluid dynamics and transfer phenomena [15], and even though there have been significant advancements to understand the local flow behaviors of the device [34, 83, 84], there remains a lack of knowledge related to the specific flow features as well as the exergy exchanges/dissipation occurring within the flashing CO₂ ejector and their relation with the operating conditions and the global cycle performance

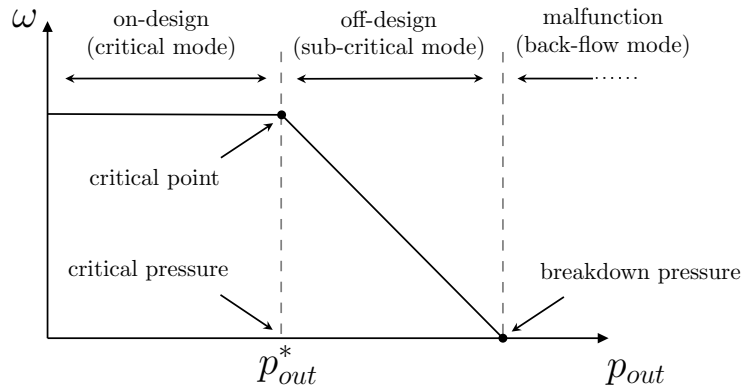


Fig. 1.3 Typical characteristic curve of an ejector.

[129, 142]. A better understanding of those phenomena is a necessity to develop more reliable design methods and obtain higher ejector efficiency and, consequently, enhanced system performance. To this end, numerical modeling constitutes a precious tool to study and design the ejector [55, 82]. The following sections constitute a brief literature review concerning the aspects of numerical modeling that are relevant within the context of the present thesis: ejector thermodynamic modeling (Section 1.2.2), modeling of ejector refrigeration systems (Section 1.2.3), computational fluid dynamics of ejectors (Section 1.2.4), and challenges relating to the validation of numerical results (Section 1.2.5).

1.2.2 Ejector thermodynamic modeling

The first one-dimensional mathematical model of an ejector was introduced by Keenan *et al.* [77] in 1950. The model was based on the application of mass, momentum, and energy conservation equations, with the use of isentropic flow relations. This model has been used as a theoretical basis in ejector design since then, as ejector models have progressively integrated more physics [125]. Since such kind of model revolves around thermodynamic principles and conservation laws applied between discrete cross sections of the ejector, they are commonly referred to as thermodynamic or 0D models [72]. Lacking information about the internal flow physics at play, the early model of Keenan *et al.* [77] assumed that both primary and secondary streams had the same pressure at the primary nozzle exit section and was thus unable to provide information about the choking phenomena [72]. The flow structures within the single-phase ejector have since been well described in the literature [23, 54, 82]. Notably, Fabri and Siestrunk [54] were among the pioneers to describe the double-choking phenomenology within an air ejector. Based on the results of shadowgraphy techniques,

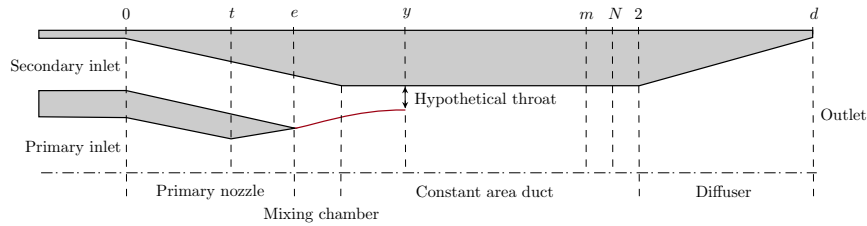


Fig. 1.4 Layout of a typical ejector with discrete sections (labeled from 0 to *d*) used in a thermodynamic model.

the authors theorized two choking behaviors depending on the secondary fluid inlet pressure. If the latter is sufficiently high, the secondary stream reaches sonic conditions and chokes at the axial position of the primary nozzle exit as it comes into contact with the primary stream. For lower secondary inlet pressures, the secondary stream reaches the speed of sound and chokes at a particular section located within the mixing chamber or mixing duct, as the primary stream expands and creates an aerodynamic (or hypothetical) throat with the ejector wall (Fig. 1.4). This latter choking phenomenology is referred to as the *Fabri-choking* and has been widely used as an hypothesis for numerous subsequent theoretical ejector models [6, 30, 33, 49, 74, 116, 131, 135, 143].

Yet, following the work of [54], the Fabri-choking has only been observed and reported, to the best of the author's knowledge, in Lamberts et al. [84], where the authors performed Schlieren imagery within a rectangular air ejector. According to Lamberts [82], in many studies, no apparent sonic section is observed in the core of the secondary stream operating under on-design regime. Building on this conclusion, Lamberts et al. [85] described a new choking theory for perfect gas based on the early work of Bernstein et al. [14] on the so-called *compound-choking* theory. This theory describes the choking phenomenology of a multi-stream flow. Unlike in the conventional approach of choking, that assumes that all streams must reach sonic velocities, the compound-choking is based on the propagation of a compound-wave and predicts that the flow may be choked even as some streams remain subsonic [14]. Comparing the results of their model with R141b experimental data, the entrainment ratio was found to lie within a 10% error range. However, like many other thermodynamic models [37, 74, 131, 135], the model of Lamberts et al. [85] remained limited to on-design entrainment ratio predictions for single-phase ejectors. On the one hand, several models were implemented to adequately handle two-phase flows by introducing the fluid quality to compute density, enthalpy, and entropy [6, 33, 72, 137]. As pointed out by Ameer et al. [6] the speed of sound in a fluid with phase change is difficult to determine accurately, especially when the phases exhibit large velocity and temperature differences. Hence, the authors implemented a method to maximize primary and secondary mass flow rates without the need to impose a unity Mach number at the throat. On the other hand, next-generation models were developed to predict both on- and off-design regimes [30, 31, 143]. The model of Chen et al. [30] was among the first to allow the prediction of the ejector performance under all operating regimes for real gas (including two-phase) ejectors. Their model

assumed the presence of the hypothetical throat inside of a constant area mixing duct for both operating regimes, and the off-design performance was obtained by using a mixing efficiency dependent on the back-pressure of the ejector. By combining different aspects of the models of Ameer et al. [6], Chen et al. [30] and Lamberts et al. [85], Metsue et al. [110] introduced a thermodynamic model of the latest generation with real-gas thermodynamic properties retrieved from the COOLPROP library [13] and the compound-choking theory for the predictions of double-choking. Five efficiencies were implemented to model friction and dissipation losses, which allowed to fit the model to accurately represent the physics. As in the model of Ameer et al. [6], the speed of sound was not required as an input, and the authors demonstrated that the use of the compound-choking criterion actually leads to the maximization of the total mass flow rate within the ejector. The article of Metsue et al. [110] is given in full length in Appendix C. While the ejector model of Metsue et al. [110] reported accurate predictions compared to experimental measurements, it was used as a standalone tool. However, it should be integrated/coupled to a model of an entire refrigeration cycle to gain more insightful knowledge. This matter is further discussed in the following section.

1.2.3 Modeling of CO₂ ejector refrigeration systems

Within the refrigeration cycle, ejectors can be used in various configurations that are well described in Besagni et al. [17] and Tashtoush et al. [141]. Of particular relevance for the present research is the transcritical CO₂ Ejector Refrigeration System (ERS), displayed in Figure 1.5. This configuration was first proposed by Gay [62] in 1931, and it has since been demonstrated to yield the highest Coefficient Of Performance (COP) and exergy efficiency among the proposed layouts for CO₂ systems [142]. In this cycle, the high-pressure CO₂ coming from the gas cooler is expanded in the ejector. The vapor coming from the evaporator is entrained within the device and pre-compressed through viscous shearing and suction induced by the high-pressure stream. At the ejector outlet, the refrigerant has an intermediate pressure, so the compressor can operate at a lower charge compared to the classical cycle. In addition, the ejector can improve the evaporator performance due to the consequently near-liquid feeding operation [123], since liquid and vapor phases are separated in the separator. Overall, the electrical consumption of the compressor is less for the same cooling/heating capacity; the COP of the cycle is thus higher.

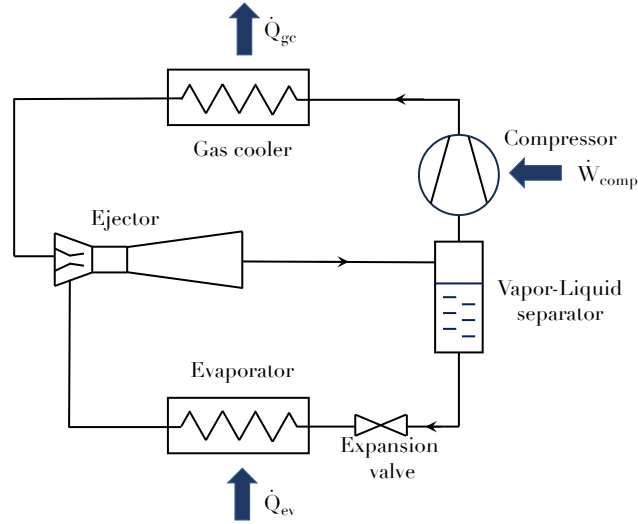


Fig. 1.5 Layout of a typical CO₂ ejector refrigeration system.

The modeling of the ERS in its entirety has been and remains to this day an ongoing subject of research used to design the ERS, predict its performance, and simulate its operation [4]. Kornhauser [80] performed in 1990 a first analysis of the ERS performance through a simple in-house thermodynamic model. The author compared the performance of a standard vapor compression cycle (without ejector) with that of the ejector cycle for different refrigerants and found potential COP improvements ranging from 12% to 30%. Using similar methods, Nehdi *et al.* [118] found that a maximum COP improvement of 22% could be achieved by using an ejector in R141b systems. Likewise, Li and Groll [87] found that the COP of the CO₂ ERS could be improved by more than 16% over the basic transcritical cycle for typical air conditioning operation conditions. Zhang and Thian [151] found that the total exergy losses of the transcritical CO₂ ejector cycle were reduced by about 43.0% with respect to the basic cycle. Several similar studies have been subsequently performed to investigate and assess CO₂ ERS performance [44, 58, 81, 153].

Because refrigeration cycles can be cumbersome to implement, adding to the fact that in-house models are not very modular, some recent studies have opted to use the Dymola commercial software as a modeling tool [32, 67, 92, 96]. Dymola is a solver based on the Modelica language that

can be coupled with relevant libraries to simulate a variety of systems, including thermal systems. Metsue et al. [109] implemented their in-house ejector model ([110]) within Dymola and investigated the influence of ejector geometry on the performance of a transcritical CO₂ ejector cycle. After calibrating the ejector model onto the CO₂ experimental data of Zhu et al. [155], the authors found that there exists an ejector size that maximizes the COP of the cycle and that the critical ejector pressure is not reached at this optimum COP point. Instead, the maximum COP was found when the ejector operated under the on-design regime, at an outlet pressure below that of critical operation. The article of Metsue et al. [109] is given in full length in Appendix D.

It should be noted at this stage that many studies dealing with the simulation of ERSs in the open literature use a rather coarse approach towards the modeling of the ejector itself, where often the on- and off-design regimes are not distinguished [109]. Consequently, little knowledge can be gained about the link between the ejector flow behavior and the performance of the ERS. Particularly, there has been no clear association of the performance of the cycle to the operating regime of the ejector (on- or off-design). Gaining this knowledge would nonetheless lead to improvements in the ejector design and the control of the ERS, both leading to a higher COP.

1.2.4 Computational fluid dynamics of ejector flows

To learn more about the internal physics at play within a supersonic ejector, Computational Fluid Dynamics (CFD) became in the early 2000's a compelling research tool, propelled by the development and availability of high computational power infrastructures [11, 12, 48, 73, 128]. Several works have then been done to characterize the flow topology with respect to the operating conditions (e.g., [61, 84]) or to study the mixing chamber geometry, shock wave formation, irreversibilities, and exergy transfers [48, 83, 147, 148]. In particular, Lamberts et al. [83] extended the transport tube analysis of Meyers and Meneveau [114] to exergy transport tubes in the context of ejectors flows. This analysis allowed to determine the locations and amplitudes of the local exergy transfers and losses within the ejector. This analysis was performed on the CFD results of a single-phase (air) ejector, and never applied, to the author's knowledge, to two-phase flows. Additionally, even though the analysis performed by Lamberts et al. [83] highlighted that the net exergy gain of the secondary stream was maximum when the ejector operated close to critical operation, this conclu-

sion remains based on the study of a single characteristic curve where a restricted number of CFD points were considered. The net exergy gain of the secondary stream has never been studied for an ejector working within an ERS, where its operating conditions diverge widely from the particular ones (constant inlet conditions) considered in [83].

While work on single-phase ejector Large Eddy Simulation (LES) has already begun [25, 35, 43], a LES of a CO₂ ejector has never been published so far. Actually, the overwhelming majority of CFD papers on ejectors was performed using Reynolds-Averaged Navier-Stokes (RANS) simulations [36, 61, 63, 89, 100] (or, rarely, Favre-Averaged Navier-Stokes (FANS) simulations in the case of density-based compressible solvers [83]), that are statistically-averaged models that rely on a turbulence closure scheme. As underlined by Ringstad *et al.* [129], accurate multiphase flow modeling is generally considered the most challenging aspect of CO₂ ejector modeling. Several strategies can be adopted to model two-phase flows. One can first distinguish pseudo-fluid models, for which the equations of both phases are averaged into one, from proper two-fluid models, where one set of the Navier-Stokes equations is solved for each phase [101, 129]. Note that, to the best of the author's knowledge, there has been no attempt to apply a two-fluid model to transcritical CO₂ ejectors. Then, one may differentiate between models based on whether they assume mechanical (i.e., velocity and pressure) and/or thermodynamic (i.e., temperature) equilibrium between the two phases. The most common approach, the Homogeneous Equilibrium Model (HEM), considers both mechanical and thermodynamic equilibria and has been extensively used to model CO₂ ejector flows [57, 93, 103, 122, 129, 139] as it provides the simplest approach toward two-phase flow modeling. This approach allows to define the state of the vapor-liquid mixture with only two independent parameters (e.g., the density and specific internal energy) through the Equation of State (EoS) [28]. In 2015, Palacz *et al.* [122] investigated the accuracy of the HEM depending on the operating conditions of the CO₂ ejector. The authors found that the HEM could accurately predict motive and suction mass flow rates for primary inlet conditions close to or above the critical point (i.e., for tested conditions with pressures between 70 and 95 [bar] and temperatures between 25 and 35 [°C]), with a relative error inferior to 10%. However, the accuracy of the HEM quickly drops as the motive pressure decreases, reaching motive mass flow rate discrepancies of 59.43% for highly subcooled inlets. Those errors were attributed to metastability effects that were not taken into account by the HEM.

Building on the conclusion drawn by Palacz *et al.* [122], metastability effects should be taken into account for the modeling of flashing CO₂ ejectors with low inlet temperatures. Discrepancies are mostly attributed to the thermodynamic equilibrium hypothesis rather than mechanical equilibrium [40, 105]. Hence, more advanced two-phase models have been implemented to tackle this issue by removing the hypothesis of thermodynamic equilibrium of the phases [21, 70, 89, 95]. Among the proposed non-equilibrium models, the Homogeneous Relaxation Model (HRM) is a so-called 4-equation model [40] that was first proposed by Bilicki *et al.* [18]. Rather than considering that equilibrium is instantly reached between the vapor and liquid phases, like in the HEM, the HRM treats phase change as a relaxation process toward the equilibrium vapor quality. Following their previous work [122], Palacz *et al.* [121] compared, using CFD tools, the validity of the HRM under different operating conditions of the CO₂ ejector and reported errors with the HRM that were approximately 5% lower than that of the HEM. Yet, the accuracy of the model remained dependent on the operating conditions, and Haida *et al.* [70] thus proposed optimized correlations for the relaxation time, based on the formulation initially proposed by Downar-Zapolski *et al.* [46] for flashing water and later adapted by Angielczyk *et al.* [8] for CO₂. Three operating ranges were defined according to the motive nozzle pressure in order to minimize the discrepancy between CFD and experimental results. Consequently, the modified HRM of Haida *et al.* [70] offers the same accuracy as the HEM in the supercritical region while benefiting from the better performance of the HRM in the sub-critical region. Recently, the HRM was used in 1D by Log *et al.* [98] to study non-equilibrium effects within the CO₂ pipe depressurization with an alternative formulation for the modeling of the relaxation time, which was defined as a function of the relative initial entropy.

Another important aspect of any CFD simulation is the equation of state (EoS) used to compute fluid properties at vapor, liquid, supercritical, two-phase equilibrium, and metastable states. It has been demonstrated by Raman and Kim [126] that the computation of these properties can strongly influence the results of CFD simulations. However, it is essential to ensure that the computation time for the EoS remains reasonable. De Lorenzo *et al.* [41] identified three approaches to achieve this goal: using a simple EoS, employing an iterative algorithm with an accurate EoS, or utilizing tabulated methods. Several early attempts were made to perform CFD of two-phase CO₂ with analytical EoSs such as the perfect gas (PG) EoS [139], the stiffened gas (SG) EoS [104, 115], or the Peng-Robinson (PR) EoS [27].

However, as pointed out by Fang [55], those are not suited for predicting such complex mixtures, which contain a wide range of thermodynamic states. It is widely accepted that the currently most accurate EoS for CO₂ is the Span-Wagner (SW) EoS [140], which is based on hundreds of parameters that are fitted by extensive experimental data [55]. This EoS has been implemented into the REFPROP [86] and COOLPROP [13] thermophysical property libraries. Despite its high accuracy, the SW EoS requires high CPU times, which is the main reason why so-called tabulated EoSs are being preferred and have been adopted in several studies [5, 57, 59, 64, 132]. With those methods, the time-consuming iterative procedure for the EoS is performed in pre-processing to create tables that are used during the CFD simulation itself by interpolating the tabulated values. Notably, Fang et al. [56] developed a lookup table for CO₂ by adapting previous work done by De Lorenzo et al. [41] for water. The tabulated method showed good accuracy, with a maximum pressure discrepancy of 0.23% with the original SW EoS. It was then coupled to an OpenFOAM solver to simulate transcritical CO₂ ejector flows, and a speed-up factor of about 66 compared to the original SW EoS was reported by the authors [57]. The table of [56], despite its notable performance, is however limited to a bilinear interpolation scheme, and of the SW EoS for CO₂ only. Moreover, the tabulated EoS is implemented as a Fortran routine, which must then be coupled to the solver as a static library, contributing to its lack of portability. To further reduce the CPU time of the CFD simulations, wall models are typically used to reduce the number of grid elements required in the near wall region and rely on simplified assumptions about flow behavior near the wall. However, those may not accurately represent the intricate dynamics of two-phase compressible flows [69]. To the author's knowledge, there has not been any record of the validation or specific implementation of a wall model suitable for flashing CO₂ flows in the open literature. However, without thorough validation against experimental or high-fidelity numerical data, it is difficult to ascertain the accuracy and reliability of predictions obtained using wall models for such simulations. Yet, many CFD studies rely on such wall models [55]. To alleviate this problem, performing wall-resolved simulation is an appropriate alternative to the use of current wall models, coming however at a significantly higher cost (and can even be prohibitive) in terms of numerical resources since the mesh must be refined at the wall in order to accurately capture the velocity gradient and shear stresses [55]. To cope with the high CPU times, implicit time integration schemes can be employed in FANS, which practically enable faster convergence of

the solution than explicit schemes. Implicit schemes are, however, more elaborate in their implementation, requiring complex derivative terms [119], which is why most of them are not compatible to solve compressible two-phase flows.

Because ejector flows are highly compressible, a density-based approach is generally regarded as more suitable compared to a pressure-based one [55]. Note that a thorough analysis of this matter is, to the best of the author's knowledge, still lacking in the open literature. There are however reports of a noticeable gain in speed for compressible cases with a density-based solver, which is also less diffusive than the pressure-based one [22]. Nonetheless, most of the CFD-HEM ejector simulations reported in the open literature use a commercial pressure-based solver (ANSYS Fluent) [36, 61, 65, 122], and to the best of the author's knowledge, a density-based solver has never been used to perform CFD-HRM simulations.

1.2.5 The challenges of experimental validation

CO₂ ejectors are made of small parts that may often be difficult to manufacture accurately, as the typical primary nozzle throat has a diameter of around 1 [mm] [63, 68, 120, 155, 156]. Along with this comes the problem of accurate measurements: (i) of the actual dimensions of the device, that should be verified after manufacturing since even a small deviation from the reference dimensions may have a drastic impact on the actual operation and hence on the numerical predictions; (ii) of the local pressures/temperatures. The relatively large size that the probes or taps may have compared to the local diameter within the ejector [90] might not allow for an accurate measurement or may even induce additional losses. Due to the geometry of the ejector, it is also particularly challenging to measure such quantities within the nozzle or even in the mixing chamber, and in any case, it is limited to wall measurements [4]. As for the inlet conditions, the probes should ideally be placed at the very inlets/outlet of the device, matching boundary conditions at the computational domain, which is in practice difficult to achieve, and there may well be additional head and/or heat losses between the probes and the actual inlets/outlet. Furthermore, experimental visualization studies of CO₂ present their own challenges (e.g., seeding), which are also aggravated by the small dimensions of the ejector compared to more regular-sized components [90, 120].

Ejectors working with refrigerants are most often operated within a thermodynamic cycle, where the refrigerant is recirculated in a closed loop. This

is because it may not be economically or ecologically allowable to simply discharge it within the ambient, and because it would be difficult to control both temperature and pressure without a cycle. This brings along another set of challenges. The first one is the presence of lubricating oil within the loop, which could affect both the measurement of the refrigerant mass flow rates and the local flow features within the ejector, such as boundary/shear layers and flow topology [39, 154]. It is expected that the lubricant dissolved in the refrigerant CO₂ builds a thin layer at the walls and that an oil mist is present in the bulk flow [134], with droplets that are expected to decrease the ejector efficiency [37]. Moreover, because the viscosity of the mixture will be higher than that of the pure refrigerant, increased friction at the walls and in the primary/secondary shear layer is expected, ultimately leading to decreased mass flow rates. Secondly, operating the inlets/outlet of the ejector independently for a deep analysis of the operating regime requires more advanced conceptions of the ERS. Hence, most studies focused on the effect of the ejector on the cycle rather than on the fine characterization of the ejector [3, 4, 52, 141]; to study the ejector, the cycle should be designed to serve the ejector and not the other way around. All those factors consequently make the validation of the counterpart numerical results more difficult, as they can generally not be taken into account when performing numerical simulations of a standalone ejector or are studied separately. The numerical simulation tool may well be quite accurate (in the sense that it can reproduce the physics accurately), but if it cannot be compared to some experimental measurements that are truly representative of what was simulated (e.g., if there is oil mixed in the refrigerant), the validation of the numerical tools may not be done in a proper way.

1.3 Positioning of the research work and objectives

From previous considerations, one may outline the fact that although CO₂ ejector systems have already been commercialized, there is still some way to go further and demonstrate that those systems can constitute a fully viable economic solution to substitute conventional systems. The numerical modeling of ejectors, whilst playing a significant role in design and performance prediction, still requires additional work, this being especially true for two-phase ejectors [4]. Additionally, one can note that works on ejector flows stimulate more fundamental research into turbulent, compressible two-phase flows with shock/boundary layer interactions and non-equilibrium effects. In this sense, this research also contributes to the improvement of

the tools and methods and broadens the knowledge related to those fields. Because of the absence of validation of current wall models on transcritical CO₂ flows, performing wall-resolved simulations constitutes a preferred approach in FANS but requires high computational resources because of the mesh refinement near the wall, which also sets constraints on the time step for explicit schemes. Implicit schemes do not suffer from the same constraints, but to the author's knowledge, there is no record in the literature of an open-source implicit FANS solver that may be compatible with solving two-phase compressible flows. Moreover, most of the recent CFD ejector simulations have been performed using the pressure-based solver of ANSYS Fluent, even though a density-based solver is arguably more appropriate. Furthermore, numerous studies have opted to deeply investigate the ERS either at the system scale or at the component level, but few have chosen to bridge the gap between these two approaches [16]. There remains a significant gap in understanding the correlation between the ejector operation (or operating regime) and the overall cycle performance. The local exergy transfers occurring within the flashing CO₂ ejector have not been studied thoroughly with the exergy tube analysis, as in single-phase, and have never been associated to the performance of the ERS. Additionally, despite the development of advanced two-phase models to account for metastable phenomena, such as the HRM, the impact of metastability on local exergy transfers and destruction has never been tackled, nor has its impact on cycle performance. Understanding those dependencies is nonetheless essential for establishing efficient design strategies at the component level and determining appropriate cycle operation strategies.

From the above concerns emanate the following research questions:

What is the impact of metastability on the performance of both the ejector and the ejector-based refrigeration system? What should be the main ejector design objectives and operation of the refrigeration system to achieve optimal performance? How are the local exergy transport phenomena within the ejector linked to the overall performance of the refrigeration system?

To answer those questions, the following objectives are set:

1. Adapt a density-based FANS CFD model to reach the same level of maturity, using the homogeneous equilibrium hypothesis, that exists for single-phase ejectors [82]. Such a model should be able to perform

wall-resolved computations of a full ejector with no prohibitively large CPU times by using an implicit time integration scheme.

2. Implement a HRM for the first time in a density-based solver to study the effects of metastability within the transcritical/subcritical CO₂ ejector. An efficient and accurate tabulated EoS, including metastable liquid properties, should be implemented with the aim to reduce as much as possible the CPU time associated to it.
3. Implement a numerical model of an ERS that includes an accurate ejector thermodynamic model to predict ERS operation, study the operating regime of the ejector, and determine what should be the main ejector design objectives to reach an optimum COP.
4. Implement the method of exergy tube analysis for two-phase ejectors as for the case of single-phase ejectors [83] to investigate transport phenomena between the primary and secondary streams and determine if there is a correlation between the optimal exergy transfers within the ejector and the performance of the ERS.

1.4 Structure of the manuscript

The following sections contain the original contributions of the present thesis, where each chapter constitutes a journal article that has either been published or submitted. Note that Appendix A summarizes all journal and conference articles that have been published/submitted during this thesis.

Chapter 2 presents the first implementation of a HRM within a density-based CFD solver. The open-source SU2 solver is chosen since it is suited to handle non-ideal cases (i.e., the Navier-Stokes equations are implemented without any perfect gas assumptions). A novel tabulation algorithm for the EoS based on piecewise bi-cubic interpolation is presented, which enables fast and accurate predictions of the standard and metastable properties. The HRM is compared to the HEM and validated against experimental wall pressure measurements from the literature. This chapter addresses points 1 and 2 of the objectives (Section 1.3). It represents the first mandatory step to build and validate the numerical tool, which is later confidently used to model the flows and associated transfers in two-phase ejectors working with carbon dioxide. The related article is published in the *International Journal of Refrigeration*.

Chapter 3 presents the second level of modeling developed during this thesis. A new generation reliable thermodynamic ejector model, based on the compound-choking theory to predict double-choking operation, is coupled to a CO₂ ERS working in the transcritical and subcritical regimes. The purpose of the study is to determine the allowable steady-state operation of the ERS and the related ejector operating regime (on/off-design), and find the ejector parameters (geometry, efficiency) that could theoretically yield an enhanced performance of the ERS. This chapter addresses point 3 of the objectives (Section 1.3). It serves as a basis for Chapter 4, in which both models (thermodynamic and CFD) will be combined to make the link between the performances at the ejector and cycle levels. The related article is under revision in *International Journal of Refrigeration*.

Chapter 4 presents a multi-scale approach to study the interconnections between local transport of exergy inside of the ejector and global performance of the ERS. To this end, previous tools are combined: the SU2 solver developed and validated in Chapter 2 is used to perform detailed simulations with access to local variables. It is also the opportunity to assess the impact of metastability by comparing the HEM and HRM results for CO₂ ejector flows, extending the comparisons for nozzle flows done in Chapter 2. The thermodynamic modeling presented in Chapter 3 is fitted onto CFD results and used to predict the operation of the ejector/cycle. This chapter addresses point 4 of the objectives (Section 1.3) and represents the main outcome of this thesis. The related article is under revision in *Energy*.

Chapter 5 ends the manuscript with a summary and discussion about the main findings of this thesis, followed by future perspectives.

In addition to the main sections of the thesis, Appendix B provides supplementary analyses related to the contents of Chapter 4, Appendix C contains a thorough description and validation of the ejector thermodynamic model used in Chapters 3 and 4, and Appendix D constitutes an application of the thermodynamic model to a real cycle using the Dymola software.

2

A Homogeneous Relaxation Model Algorithm in Density-Based Formulation with Novel Tabulated Method for the Modeling of CO₂ Flashing Nozzles

2.1 Foreword

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Title: A Homogeneous Relaxation Model Algorithm in Density-Based Formulation with Novel Tabulated Method for the Modeling of CO₂ Flashing Nozzles.

Abstract:

Accurate prediction of the flow physics within nozzles and ejectors working with two-phase carbon dioxide remains particularly challenging. Indeed, the flashing phenomenon in the device often comes along with the formation of the metastable phase, which can severely affect both the flow physics and the flow rate. Due to the particular challenges associated with building and operating two-phase carbon dioxide experimental setups, computational fluid dynamics constitutes a compelling alternative to predict and study nozzle and ejector flows. In this work, the metastability effects are modeled through a Homogeneous Relaxation Model for the first time expressed in density-based formulation, within the SU2 solver. The thermodynamic relations for the equation of state are tabulated using a novel quadtree algorithm and directly coupled to the solver, ensuring fast and accurate predictions. The simulation tool is then validated against experimental nozzle pressure profiles and used to compare the commonly used Homogeneous Equilibrium Model to the Homogeneous Relaxation Model in terms of local flow topology and mass flow rates. Most notably, it was found that the Homogeneous Relaxation Model was able to better fit the experimental pressure profiles within the first part of the expansion.

2.2 Introduction

Carbon dioxide (CO₂) has emerged as a suitable alternative to conventional refrigerants owing to its minimal impact on climate change. With a noteworthy combination of attributes, including a zero ozone depletion potential

(ODP) and a global warming potential $\text{GWP} = 1$, CO_2 has garnered substantial attention from the industry. Particularly in the context of refrigeration and heat pump systems, CO_2 stands out as an attractive working fluid due to its non-toxic and non-flammable nature, adding to the fact that transition towards CO_2 utilization has been necessitated by international agreements such as the Kyoto Protocol, which outlined phased reductions in the usage of HydroChloroFluoroCarbons (HCFCs) by 2020-2030 and HydroFluoroCarbons (HFCs) by 2025-2040 [2]. More recently, the European Commission reviewed the F-gas regulation with the intent to reduce the EU's fluorinated greenhouse gases emissions by two thirds by 2030.

The particular thermodynamic properties of CO_2 , with a critical temperature of $31\text{ }^\circ\text{C}$, require the operation of the cycle under transcritical conditions. However, it introduces considerable losses in the expansion valve due to the high pressure ratio [79] and the entropy production during the isenthalpic expansion. Devices such as ejectors are then the subject of many researches, as they can be used to partially recover the expansion losses into useful mechanical work. Nonetheless, ejectors are notoriously characterized by complex fluid dynamics, and some of the underlying mechanisms within these devices remain insufficiently understood, impeding overall system performance [15]. One particular aspect adding to this complexity is the emergence of the metastable phase during the flashing of the flow within the primary nozzle of the ejector. In such highly compressible flows, the phase change significantly depends on the rate of bubble nucleation [124]; the decompression is so fast, inducing high velocities and low residence time, that the fluid does not have sufficient time to reach equilibrium and then vaporize under the usual saturation conditions. Consequently, there is a delay before the flow returns to the liquid-vapor equilibrium state. This practical implication results in distinct flow topologies, thermodynamic states, and higher mass flow rates than equilibrium conditions. Addressing, predicting and understanding these aspects is then crucial to correctly model two-phase CO_2 ejectors, as the correct modeling of the primary stream issued from the nozzle is the key to further predict the correct entrainment capability of the ejector.

Design of nozzles and ejectors is often achieved using numerical tools. Thermodynamic models are fast and allow to predict the operation of the device for a wide range of conditions to determine the main geometric parameters. The design can then be refined through a Computational Fluid Dynamics (CFD) analysis that also allows access to local flow features. It enables a deeper analysis of the influence of the geometry on the device's operation.

Experimental campaigns, despite being associated with challenges related to high pressures (within the range 50 - 100 [bar]) and small dimensions of the components (nozzle diameter of about 1 [mm]), are then necessary in order to calibrate 1D models and validate the CFD results. Reynolds-Averaged Navier-Stokes (RANS) models for incompressible (or weakly compressible) flows and Favre-Averaged Navier-Stokes (FANS) models for compressible flows are statistically averaged models that rely on a turbulence closure scheme. Because of the prohibitive computation times associated to direct or large eddy simulations, most two-phase nozzle and ejector simulations performed up to now are based on RANS or FANS closures. Most studies that have been undertaken to perform CFD of two-phase CO₂ ejectors [63, 64, 70, 121] were done using the commercial software ANSYS Fluent [9], using a pressure-based solver. However, as pointed out by Fang [55], density-based flow solvers are more suitable for computing compressible flows.

As underlined by Ringstad et al. [129], accurate multiphase flow modeling is generally considered as the most challenging aspect and the key factor for successful modeling of CO₂ ejectors. Complex interactions take place between the vapor and liquid phases, adding to the fact that the flow flashes into the primary nozzle in the case of transcritical CO₂ operation. There are several model hierarchies to handle two-phase flows according to the type of equilibrium (mechanical, thermal, chemical) that is assumed to be relaxed [40]. One can distinguish pseudo fluids, for which the equations of both phases are averaged into one set of the mixture equations, from proper two-fluid models where one set of equations is solved for each phase. The widely adopted approach, known as the *Homogeneous Equilibrium Model* (HEM), characterizes the flow as a pseudo fluid in mechanical, thermodynamic and chemical equilibria. More sophisticated approaches include the *Homogeneous Relaxation Model* (HRM) or the *Delayed Equilibrium Model* (DEM), that are so-called 4-equation models that assume only mechanical equilibrium [129]. The HEM has been extensively used to model CO₂ ejector flows [57, 93, 103, 122, 129, 139] as it provides a simplistic approach toward two-phase flow modeling. This allows to define the state of the vapor-liquid mixture with only two independent parameters. Palacz et al. [122] investigated the accuracy of the HEM depending on the operating conditions of the CO₂ ejector. It was found that the HEM could accurately predict mass flow rates for primary nozzle conditions close or above the critical point (i.e., for tested conditions with pressures between 70 and 95 [bar] and temperatures between 25 and 35 [°C], roughly), with a relative error inferior

to 10%. However, the accuracy of the HEM quickly drops as the motive temperature decreases, reaching motive mass flow rate discrepancies up to 59.43%. Those errors were attributed to metastability effects that are not taken into account by the HEM. Metastability effects should be most present as the inlet temperature gets lower since the expansion path is expected to cross the saturation curve at lower pressures, where the range of possible metastable states is larger.

Building on the conclusion drawn by Palacz *et al.* [122], metastability effects should be taken into account for the modeling of flashing ejectors with low inlet temperatures. To do so, an additional transport equation for the vapor fraction with a phase change model is needed [129]. As the DEM is mostly limited to 1D simulations since it requires a 1D semi-empirical relation to model the saturated mass fraction evolution along the direction of the expansion, the HRM constitutes a compelling approach for modeling metastability. Initially proposed by Bilicki *et al.* [18], the HRM diverges from the instantaneous equilibrium assumption made in HEM and treats phase change as a relaxation process towards the equilibrium vapor quality. Downar-Zapolski *et al.* [46] presented a correlation for the relaxation time and validated it in the case of flashing water. Angielczyk *et al.* [8] extended the closure law for CO₂. Their 1D HRM results were compared to available experimental nozzle data [117] and a reasonable agreement was found downstream of the throat. Haida *et al.* [70] later investigated the performance of the HRM and deduced correlations for the relaxation time for CO₂ from genetic algorithm optimization, and three operating ranges were defined according to the motive nozzle pressure, in order for the related set of empirical coefficients to minimize the discrepancy between CFD and experimental results. Recently, the HRM was used in 1D by Log *et al.* [98, 99] to study non equilibrium effects within CO₂ pipe depressurization.

Another important aspect of any CFD simulation is the equation of state (EoS) used to compute fluid properties at vapor, liquid, supercritical, two-phase equilibrium and metastable states. The work of Raman and Kim [126] has demonstrated that the computation of these properties can significantly influence CFD results. However, it is essential to ensure that the computation time for the EoS remains reasonable. De Lorenzo *et al.* [41] identified three approaches to achieve this goal: using a simple EoS, employing an iterative algorithm with an accurate EoS, or utilizing tabulated methods. Smolka *et al.* [139] presented a model of the compressible transonic single- and two-phase flow of a real fluid within an ejector. The authors validated

their model using the perfect gas (PG) EoS, both for single-phase refrigerants and for two-phase CO₂ even though the PG EoS is not suited for predicting such complex mixtures [56]. Another alternative is the Peng-Robinson (PR) EoS, used by Brown *et al.* [27] to simulate high pressure CO₂ pipelines. Note however that the PR EoS is not suitable for the simulation of two-phase flows such as flashing CO₂ nozzles, as it is invalid under the saturation dome since this EoS predicts negative speeds of sound in this region [55]. The currently most accurate EoS for CO₂ is the Span-Wagner (SW) EoS [140]. It is based on hundreds of parameters fitted using extensive experimental data. It has been implemented into thermophysical property libraries like REFPROP [86] and COOLPROP [13]. Despite its high accuracy, the SW EoS requires considerable computational resources, leading to the preference for tabulated EoSs. With those methods, the time-consuming iterative procedure for the EoS is usually performed at the beginning of the computation to create a table that will be used in the later stages of the simulation, by interpolating the tabulated values. Giacomelli *et al.* [64] constructed lookup tables in the (specific volume - specific internal energy) space from REFPROP using an in-house Matlab code, to perform ejector simulations with ANSYS Fluent. The authors implemented a bi-linear interpolation scheme to retrieve the adequate values of density and speed of sound at each cell of the domain. Ameli *et al.* [5] later implemented a similar lookup table in Fortran and coupled it to ANSYS CFX 17.0 to investigate the condensation process in transcritical CO₂ nozzles. Fang *et al.* [56] developed a similar Fortran lookup table for CO₂ by adapting the work of [41] for water. The tabulated method used bilinear interpolation and had a speed-up factor of about 66 compared to the original SW EoS. Later, Föll *et al.* [59] developed a tabulated method based on piecewise polynomials with adaptive refinement in the state space and coupled it to the Fortran CFD solver FLEXI [1]. Lastly, Rubino *et al.* [132] developed a lookup table based on unstructured grids with mesh refinement. Their method based on a bilinear interpolation scheme was coupled to the non-ideal CFD SU2 solver. They found out that an unstructured interpolation grid is beneficial in terms of computation time only when it was coarse enough.

To the best of the authors' knowledge, none of the aforementioned 2D RANS studies on HRM used a density-based solver though it is more appropriate for highly compressible flows [55]. This is most likely because the HRM is favorable to a pressure-based implementation, as discussed in the following sections. Moreover, the literature often lacks of comprehensive explanations about the computation of metastable properties, including

limitations related to the spinodal limit, that is, the limit beyond which the fluid becomes unstable (phase change must happen before reaching this limit). In this study, one introduces two novel tools for CFD modeling of compressible two-phase flows. First, a new general EoS tabulation algorithm is presented. The tabulated method combines for the first time a piecewise bicubic interpolation of the thermodynamic properties with local refinement of the interpolation grid based on a required accuracy. Secondly, a HRM is implemented within the SU2 solver [119] and directly coupled to the FANS solver. This implementation represents the first instance of expressing HRM in a density-based formulation. To validate and verify non-equilibrium phenomena within flashing CO₂ devices, good quality (CFD-grade) local measurements are needed. However, there is a clear lack of experimental data available for relevant cases (nozzles or ejectors with low inlet temperatures, that should be desired in refrigeration applications). The standard cases of Nakagawa et al. [117] despite lacking mass flow measurements, constitute, to the best of the authors' knowledge, the only set of data that is suitable to study/validate the effects of metastability within the flashing CO₂ nozzle. In this work, wall-resolved simulations of the cases of [117] are then performed using both the HEM and the newly implemented HRM to investigate and compare their predictive capabilities with respect to metastability phenomena.

2.3 Numerical methodology

In this section, all ingredients of the numerical solver are detailed. This includes geometrical modeling, multiphase models (HEM and HRM), the lookup table construction and interpolation methods to evaluate the thermodynamic properties, initial and boundary conditions, the calculation procedures and the mesh grid.

2.3.1 Geometrical modeling and operating conditions

The present study is performed using the classical cases of Nakagawa et al. [117], who considered the discharge of high pressure CO₂ through four different 2D (rectangular, with a width of 3 [mm]) nozzle geometries, that differ only by the angle of the divergent section θ . The dimensions and operating conditions of the devices are given in Table 2.1, and the nozzle schematic along with the mesh is shown in Figure 2.1. Although four geometries were presented in [117], the geometry with the highest diverging

2 | A HRM in density-based formulation

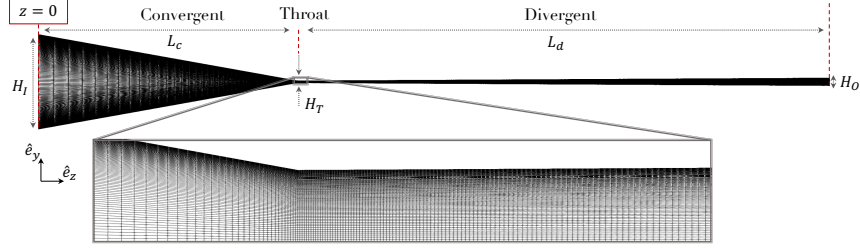


Fig. 2.1 Two-dimensional mesh for the nozzle *c* of [117] with relevant notations. The related dimensions for the different geometries are given in Table 2.1.

angle is discarded here. The reason is that, for such a configuration, the solid phase is present in the nozzle (the pressure falls below the triple point pressure during the CFD). Note that even though the geometry is 2D, 3D effects are still to be expected in the experiment, which may be the cause of some discrepancies with numerical results [82].

Nozzle	p_{in} [MPa]	T_{in} [°C]	θ [°]	H_o [mm]	H_T [mm]	H_I [mm]	L_c [mm]	L_d [mm]
a	6.1	20.5	0.076	0.39	0.24	10	27.35	56.15
b	6.1	20	0.153	0.54	0.24	10	27.35	56.15
c	6.1	21.8	0.306	0.84	0.24	10	27.35	56.15

Table 2.1 Dimensions and operating conditions of the nozzles considered by [117].

2.3.2 Numerical modeling

The FANS simulations are performed with the open-source *real-gas* SU2 (version 7.3.1) solver. The partial differential equations (PDEs) in SU2 are discretized using a finite volume method with a standard edge-based structure on a dual grid with control volumes constructed using a median-dual, vertex-based scheme. For detailed information, the interested reader is invited to refer to [119], where the FANS equations are also presented. The main numerical aspects of the code along with the particular setup used in the present work are however described in this section.

As the solver is density-based, the solution variables are $(\rho; \rho u_j; \rho e_t)$ with ρ the density and u the velocity, with the j subscript referring to the three

spatial directions. The total energy e_t is defined as:

$$e_t = e + \frac{u_j u_j}{2} + k, \quad (2.1)$$

where the t subscript indicates total quantities and k is the turbulence kinetic energy (TKE). The Menter Shear Stress Transport model [107] ($k - \omega$ SST) is used, as it demonstrated good agreement with experimental measurements, for both local and global flow quantities in the case of perfect and real gas ejector flows [36, 84].

In the present work, the convective fluxes are integrated using the classical Roe scheme [130] with second order reconstruction. The gradients of the flow variables required for the computation of the viscous fluxes are calculated using a Green-Gauss method. For HEM, an implicit Euler time integration scheme is employed, where the steady-state solver uses local time-stepping in order to accelerate the convergence. Note that by doing so, the intermediate results of the FANS simulation have no physical meaning, but the converged steady-state solution does. For HRM, the explicit Euler scheme is used for pseudo-time integration. This is because the implicit formulation requires complex thermodynamic derivatives and complex modifications in the solver that are beyond the scope of the current work.

2.3.3 Multiphase modeling

In the following, the Homogeneous Relaxation Model (HRM) is described and its differences with respect to the Homogeneous Equilibrium Model (HEM) are highlighted.

In the HEM, both mechanical and thermodynamic equilibria between phases are assumed. Consequently, using the HEM is equivalent to considering that both phases exchange mass instantaneously (through evaporation and condensation), or in other words, that the equilibrium of the phases is reached instantaneously. In practice, this hypothesis may not be true as mass exchange processes require some time to take place, and as the flow is highly compressible, the time scale of said processes may become of the same order of magnitude as the time scale of the expansion process. It is then expected that a metastable phase may appear (for example, the metastable *liquid* phase in a flashing nozzle), which could influence the flow physics in a non negligible manner. As the HEM is not able to model metastability, one may add an extra equation for the transport of the vapor phase and model the delay to reach equilibrium as a relaxation process. This

2 | A HRM in density-based formulation

approach constitutes the basis of the HRM, that belongs to the family of 4-equation models (please refer to [40] for additional details). In the HRM, the mechanical equilibrium of the two phases is kept (i.e., same pressure and velocity), but the thermodynamic equilibrium is relaxed. In practice, the fluid is then modeled as a mixture of saturated vapor and metastable liquid, and the temperature equality of the two phases is not assumed like in HEM. The additional equation needed to solve the saturated vapor phase is then modeled as:

$$\frac{\partial}{\partial t} (\alpha \rho_{sv}) + \frac{\partial}{\partial z_i} (\alpha \rho_{sv} u_i) = \Gamma, \quad (2.2)$$

with α the void fraction and Γ a phase source term. The above relation can be obtained by writing the mass conservation equation for the vapor phase over a control volume, using the definition of the void fraction $\alpha = \frac{\rho_l - \rho}{\rho_l - \rho_{sv}} = \frac{\rho x}{\rho_{sv}}$, with the l subscript referring to the liquid phase (metastable or saturated). Using the latter relation, Eq. (2.2) can be written in terms of quality as:

$$\frac{\partial}{\partial t} (\rho x) + \frac{\partial}{\partial z_i} (\rho u_i x) = \Gamma, \quad (2.3)$$

The source term Γ is then required to allow mass transfer between the two phases, as $\Gamma = 0$ implies pure convection of the phases. For the HRM, Γ models a relaxation process towards the equilibrium state:

$$\Gamma = -\rho \frac{x - x_{eq}}{\theta}, \quad (2.4)$$

where x_{eq} is the equilibrium quality and θ is the relaxation time. The latter was modeled by [46] as:

$$\theta = \theta_0 \alpha^a \Phi^b, \quad (2.5)$$

where θ_0 is the initial relaxation time, a and b are empirical coefficients and Φ is the non-dimensional pressure difference. Angielczyk et al. [8] extended the formulation of θ , initially validated in the case of water, to flashing CO₂. Additionally, the same authors [8] extended the definition of Φ to handle supercritical inlet conditions by computing the latter as a function of the inlet entropy instead of the temperature as in the work of [46]:

$$\Phi = \left| \frac{p_{sat}(s_{in}) - p}{p_c - p_{sat}(s_{in})} \right|, \quad (2.6)$$

with p_c the critical pressure and s_{in} the inlet entropy. In the following, constant θ values will be first considered to perform a parametric analysis. Then, the correlation of [8] with ($\theta_0 = 2.14 \times 10^{-7}$ [s]; $a = -0.54$; $b = -1.76$) will be applied. Note that an alternative formulation for the relaxation time was recently proposed in [98], but it was found that the values of θ obtained with this method were high and could not be applied in the present case as the spinodal limit would be reached.

As mentioned in the previous section, the HRM is favorable for a pressure-based implementation of the RANS solver. In that case, the pressure is a solution variable and it can be used directly to recompute the two-phase mixture density, as per, e.g., [70, 121], using the following mixture equations:

$$\frac{1}{\rho} = \frac{x}{\rho_{sv}(p)} + \frac{1-x}{\rho_{ml}(p, h_{ml})}, \quad h = xh_{sv}(p) + (1-x)h_{ml}, \quad (2.7)$$

with the $_{ml}$ subscript referring to the metastable liquid phase. Although the exact manner in which Eqs. (2.7) are used is not well described in the literature, it is assumed that the enthalpy equation is inverted to compute h_{ml} from solution variables (p, u_i, x, h_t), which is in turn used to compute the density. Because the present solver –SU2– is *density*-based, the same algorithm cannot be used to apply the HRM. Indeed, in this case, the density is now a solution variable, which should not be re-computed as this would lead to incoherence in the modified FANS equations. Instead, the proper way to solve this problem is to compute the pressure and total enthalpy as functions of the solution variables ($\rho, \rho u_i, \rho x, \rho e_t$). However, because saturation properties are computed as functions of pressure, which is to be calculated from solution variables, one must iterate on that said pressure to find the solution. Figure 2.2 illustrates the proposed algorithm for a density-based solver. The procedure to compute the state begins with the input of (ρ, e, x) that are either solution variables or easily computed from those. The equilibrium quantities (same as HEM) are first computed, then if the state is under the saturation dome, the HRM algorithm is used, otherwise the pressure is equal to the equilibrium pressure, that is then used to compute the total enthalpy. If two-phase is detected, the closure equations for the specific energy and the density are solved by iterating on the pressure until sufficient precision is met. In practice, a golden search-type method is used to converge on the solution pressure, with the triple and critical pressures of CO₂ as lower and upper bounds, respectively. Once the solution pressure is found, the remaining properties such as the metastable temperature T_{ml} ,

2 | A HRM in density-based formulation

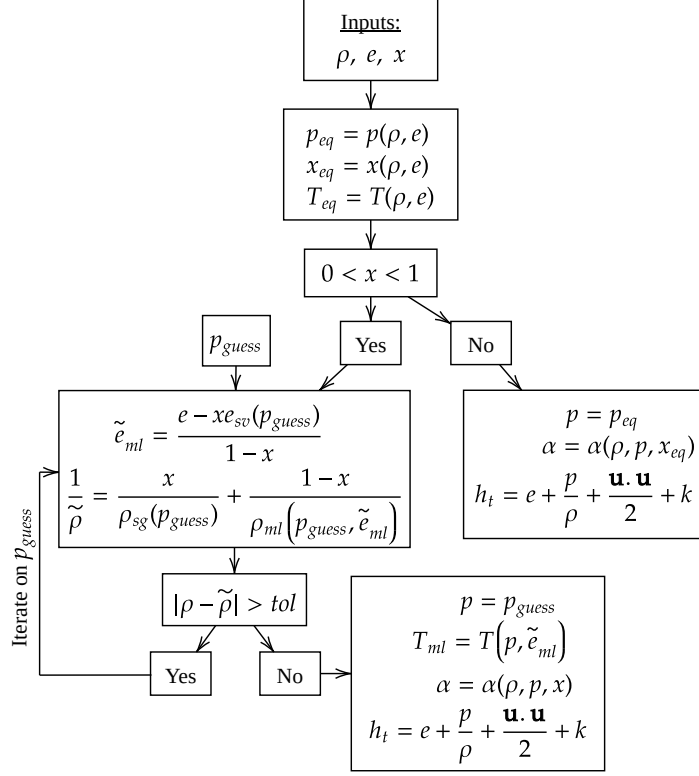


Fig. 2.2 Flowchart of the HRM algorithm in density-based formulation.

void fraction α and total specific enthalpy h_t can be retrieved directly. Note that the conduction term has then to be divided in two terms, weighted by the void fraction, to account for the contributions from both the saturated vapor and metastable liquid phases:

$$q = -(1 - \alpha)\kappa_{ml} \frac{\partial T_{ml}}{\partial z_j} - \alpha\kappa_{sv} \frac{\partial T_{sv}}{\partial z_j}. \quad (2.8)$$

2.3.4 Tabulated method

The EoS used in the present work is provided by the REFPROP/COOLPROP libraries which implement the SW EoS. As the SU2 solver was made suited to handle real-gas CFD, the state is contained within a Fluid object and the EoS is implemented in the related Fluid class. The thermodynamic

relations required by the solver must then be implemented. In this case, since the solver is density-based, the relation needed for closure is of the type $\chi = \chi(\rho, e)$, where χ is any relevant thermodynamic property. Depending on the desired features of the solver, thermodynamic relations are also required in state spaces different than $(\rho - e)$, e.g., in $(p - T)$ and $(h - s)$ state spaces for the computation of total boundary conditions, or even in $(p - e_{ml})$ to compute the metastable liquid density in HRM (Fig. 2.2).

The table is generated by a Python routine and the properties are retrieved through the Python wrapper for COOLPROP, that offers a REFPROP interface as well. By default, the properties are retrieved from REFPROP except in the case of the thermodynamic derivatives (mostly required for the implicit Euler integration scheme), that are only available in COOLPROP. These derivatives are however limited to the single-phase region and two-phase properties must be reconstructed from the saturation properties as done by [55].

Look-up table boundaries

Since the present lookup tables are generated with the aim of performing CFD of transcritical CO₂ nozzles, the state space boundaries are chosen to enclose the range in which those devices should operate. However, it is necessary to provide some margins because the numerical solver can oscillate during the solution convergence process. Figure 2.3 displays the $p - h$ diagram of CO₂ in which the blue area represents the range of states that are found in the nozzle of [117] (case c, Tab. 2.1). Those states were obtained by performing the RANS simulation in SU2 using the HEM. The theoretical isentropic expansion curve is also plotted as a reference. For this work, the table boundaries were represented in the $p - h$ diagram because it offers good readability for application in refrigeration cycles and is easy to interpret compared to less usual diagram such as the $\rho - e$ diagram. The bottom/top boundaries were chosen as 0.52/50 [MPa] (the low pressure corresponds to the triple point pressure). The left boundary is then the enthalpy of the triple point whereas the right boundary corresponds to the enthalpy at 800 K and the lowest pressure. Those boundaries apply for all tables, whether the state space is $\rho - e$ or another one. The method is however not restricted to such kind of boundaries and the user is free to implement new ones.

2 | A HRM in density-based formulation

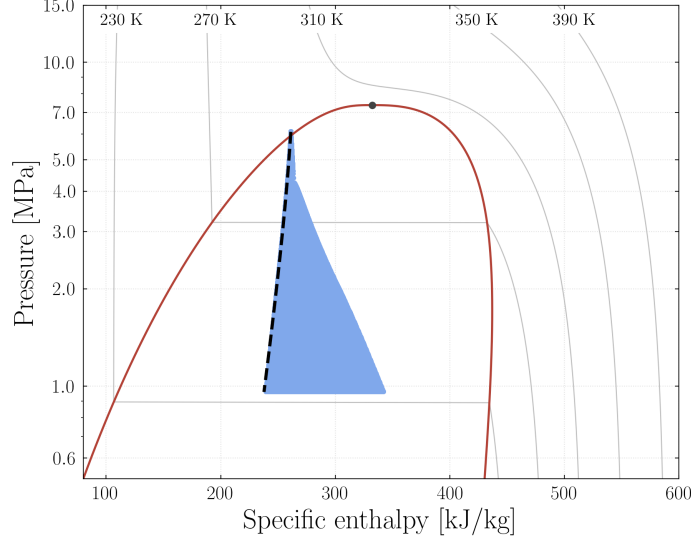


Fig. 2.3 Range of operation (in blue) of the nozzle of Nakagawa *et al.* [117] (case c, see Tab. 2.1). The saturation dome is highlighted in red with the critical point marked with the black dot. The dashed curve is the isentropic expansion, for reference.

Interpolation method

A bicubic interpolation scheme is implemented in the state space, as it was found that this method allows good precision whilst requiring limited memory storage compared to more complex approximation methods, or even the simpler bilinear interpolation. Indeed, a bicubic function reduces the amount of required cell elements by two orders of magnitude while requiring only 4 times more memory per cell, compared to a bilinear function.

The state space is discretized by a number of rectangular cells until a given absolute interpolation precision is reached for the required thermodynamic variable. The mesh generation algorithm in the state space is described in the following. Figure 2.4 displays a schematic of a cell element taken from the state space whose boundaries $(x_{l,r}, y_{b,t})$ are set as inputs by the user. Each cell is defined by its boundaries in $(x_{1,2}, y_{1,2})$ and the values at the 16 equally spaced nodes (black dots in the figure) are evaluated to calculate the bicubic polynomial:

$$F = XAY, \quad (2.9)$$

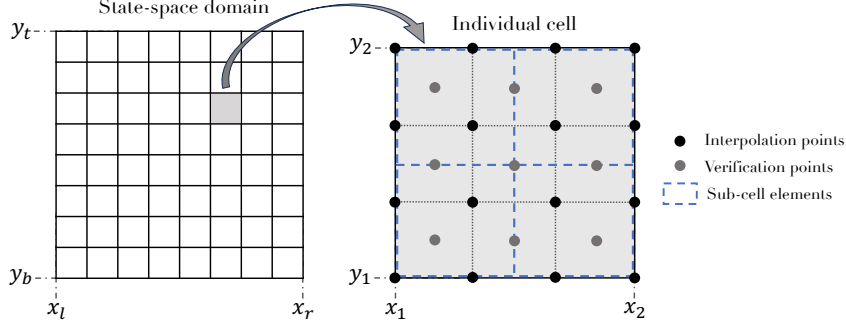


Fig. 2.4 Schematic of an individual cell taken in the state-space domain. The thermodynamic relation is interpolated on 16 equally-spaced points and the error is calculated at 9 locations called verification points.

where X is the 4×4 matrix where each line is of the form $[1, x_i, x_i^2, x_i^3]$, with the i th subscript ranging from 1 to 4, which corresponds to the abscissa of the 16 passage points (Fig. 2.4). Matrix Y is reciprocally the same for the ordinate but transposed, and $F_{ij} = f(x_i, y_j)$ is the evaluation of the thermodynamic function. The 16 polynomial coefficients A_{ij} can then be retrieved by matrix inversion:

$$A = X^{-1}FY^{-1}. \quad (2.10)$$

To speed up the generation process and avoid a loss in accuracy (due to finite machine precision) for large values of (x, y) , the cell boundaries are normalized, thereby, $X^{-1} = (Y^{-1})^T$ is constant.

During the CFD simulation, the 16 coefficients of A are retrieved from the look-up table and the thermodynamic property is computed. Note that the coordinates in the state space (x^*, y^*) must also be normalized by the cell dimensions, i.e.,

$$x^* = \frac{x - x_1}{x_2 - x_1} \quad y^* = \frac{y - y_1}{y_2 - y_1}. \quad (2.11)$$

Mesh generation algorithm

A local refinement method is implemented in the thermodynamic state space in order to limit the storage required for the interpolated quantities. In this way, more elements are generated where the function is strongly non-linear, thereby ensuring a better accuracy. This also allows the user to

set the required precision of the interpolation method to a desired value, that will be applied in the whole state space.

The mesh is generated using object-oriented programming in Python, where each cell (see Section 2.3.4) is an instance of a Cell object, that contains the cell coordinates, polynomial interpolation coefficients and cell number as attributes. Figure 2.5 presents a flowchart of the corresponding algorithm. The –recursive– routine consists in creating an instance of a Cell object that will constitute the *whole* grid. The constructor is called with specified cell boundaries (which correspond, in the case of this first cell, to the state-space domain), an absolute error tolerance for the tabulated thermodynamic property and a cell number, by default set to 0 for this first cell. The constructor then calculates matrix A with Eq. (2.10) and if the cell is within the *validity* domain or overlapping it, an interpolation error is approximated. Note at this stage the difference between: (i) the state space formed by the $(\rho - e)$ couple used to compute a third quantity, and (ii) the validity domain, that is the space in which one ensures an interpolation up to the required accuracy (in this work in the $(p - h)$ space). The interpolation error is computed by taking the maximum absolute error over 9 verification points that are located in between the 16 passage points (see the gray dots in Fig. 2.4). If the error is higher than the specified tolerance (chosen by the user), the cell is subdivided into 4 sub-cells. The constructor is then called recursively on each Cell object, and the 4 sub-cells (blue dash lines in Fig. 2.4) are instantiated as attributes of the current Cell; for each of those 4 cells, the constructor is called with a halved range, the same tolerance and a new unique cell number. This process goes until the tolerance criterion is met, then the Cell data is stored in an external text file. Each line of the text file corresponds to a cell and is composed of the cell number, its x and y boundaries in the state space, the 16 polynomial coefficients and the 4 sub-cell numbers. If the cell is at the bottom of the tree, there are no sub-cells and -1 is stored instead, which acts as a flag for the later reading process. This method essentially constitutes a quad-tree algorithm, used to find the adequate cell in which the point of interest is located (in the state space) during the actual CFD. When the cell at the bottom of the tree is reached, the 16 bi-cubic polynomial coefficients are retrieved and the function is calculated.

Limitations and fallback Methods

Because the thermodynamic relations provided by COOLPROP/REFPROP are not always able to provide a solution, e.g., near the critical point, the algorithm should be able to handle such cases without storing non-physical

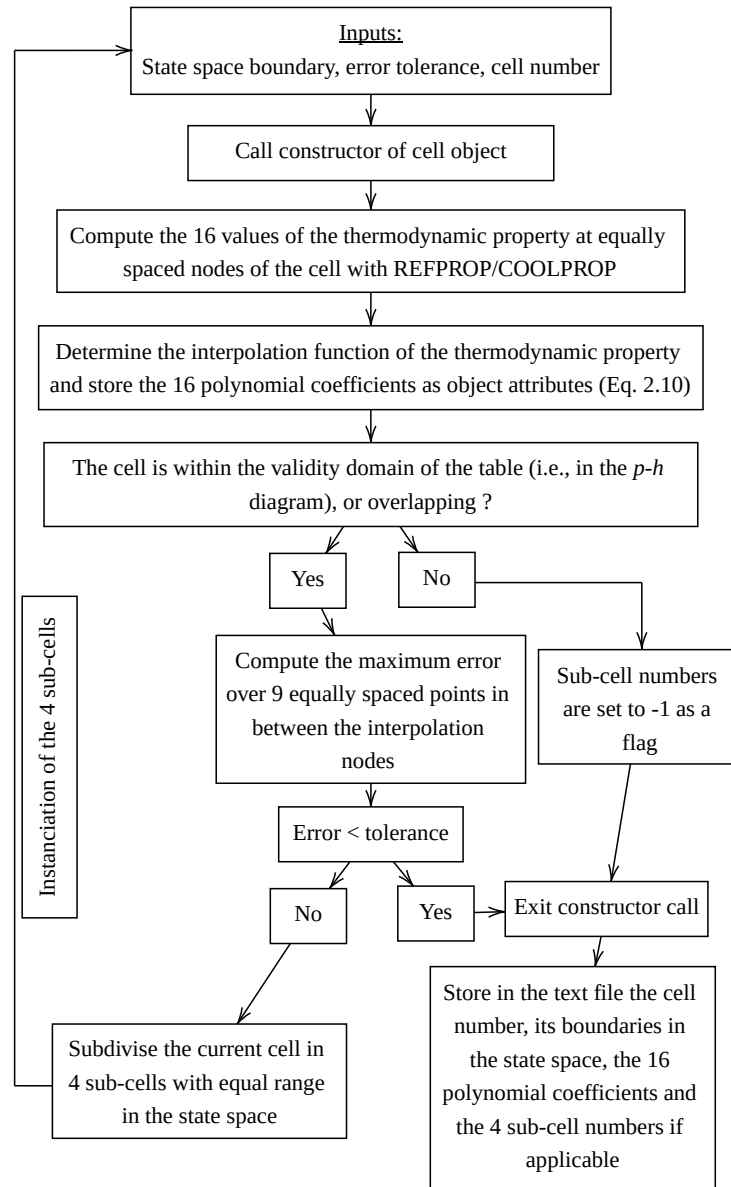


Fig. 2.5 Flowchart of the grid generation algorithm for the look-up table.

values. The strategy adopted in the present work is twofold: (i) if no value can be computed at any of the 16 interpolation points within the cell, this current cell is deleted and the lookup table falls back on the upper cell, though the precision criterion may not be met; (ii) if some values can be computed but not for all of the 16 interpolation points, the cell is further subdivided unless no values can be computed in one of its 4 sub-cells (i.e., case (i)). In addition, because there can be quite high gradients near the saturation line, one can also choose to relax the error tolerance if the cell dimensions are getting below a certain threshold, in order to avoid building a prohibitively large lookup table.

Even though those strategies relax the error tolerance, the error is located in a very small range of the state space, often located in the near vicinity of the critical point. The actual error of the generated table is thus checked a posteriori in the following section to ensure that it stays reasonable in said region. In addition, note that during the CFD simulation itself, some thermodynamic states may pass through the region of less accuracy, but usually only during the convergence process.

2.3.5 Initial and boundary conditions and numerical procedure

Total quantities are prescribed at the inlet of the nozzle, i.e., the total inlet pressure p_{in} and the total inlet temperature T_{in} , whereas the (static) pressure is specified at the outlet. Note that the inlet and outlet boundary conditions are characteristic-based (non-reflective) so that spurious reflection waves do not interfere with/impede the convergence of the solution. In practice, this weak boundary condition allows the nozzle to become fully supersonic if the specified outlet pressure is below the minimum outlet pressure allowable by the physics at fixed inlet conditions. Because the experimental cases of Nakagawa et al. [117] are fully supersonic, a low value for the outlet pressure of 0.8 [MPa] is specified, and never achieved in practice as the flow is supersonic at the outlet. A no-slip adiabatic (strong) boundary condition is applied at the wall. In addition, an extra set of boundary conditions for the quality is needed when using the HRM as Eq. (2.3) is added. For the inlet/outlet, the characteristic-based boundary condition is applied to the quality (ρx). Note that there is no need to impose a boundary condition at the wall for the quality as there is no diffusion term in Eq. (2.3).

The interior of the domain (excluding the boundaries) is initialized using pressure and density values that must be specified by the user. The inputted density is also used with the pressure to calculate the state at the outlet

during initialization. In addition, a Mach number is specified to initialize the velocity field required for the momentum and compute the total quantities at the inlet. In HRM, the quality is initialized to the equilibrium quality and the other (solution) variables are initialized with the converged HEM solution variables. The HRM simulation is then carried out until convergence. At the beginning of each iteration of the solver, the tabulated EoS is used to compute primitive variables (e.g., p , T , etc.) as a function of the density and the specific internal energy. The solution is then moved forward in time and the EoS is used once again in preparation for the turbulence model. Lastly, the turbulence properties are integrated with time.

For the HEM simulations, the CFL number is set to a constant value of 50 for 30 000 iterations, then to 5 for another 20 000 iterations in order to allow finer convergence/solution accuracy. The local time step is then computed in each cell based on this CFL, the local mesh size and velocity. For HRM simulations, slight modifications were made to the original implementation of the solver to set the CFL as a linear function of the quality, that is, $CFL = 0.05$ if $x = 0.0$ and $CFL = 0.5$ if $x \geq 0.5$. This is done because the system of PDEs becomes stiff as the quality tends towards zero (large speed of sound compared to advection velocity in the incompressible limit). Thus, the solution is propagated more quickly in the regions with higher qualities, where the relaxation process modeled by the HRM is less important. In most of the divergent part of the nozzle (far from the throat), $CFL \approx 0.5$, which contributes to accelerate the convergence process. By doing so, it was found that a solution could be obtained with roughly 5.10^6 iterations. The convergence criterion that is used is based on the conservation of the mass flow rate through the device; the solution is considered converged when the relative difference of mass flow rates between inlet and outlet steadily fell below 5.10^{-3} .

The entirety of the computation is performed on the Digital Research Alliance clusters in Canada. Each case ran on a single computation node that is comprised of 40 Intel Skylake cores operating at 2.4 GHz.

2.3.6 Mesh grid

The 2D mesh (Fig. 2.1) is generated using GMSH and refined at the wall to ensure a maximum wall coordinate $y^+ \approx 1$, a prerequisite for the $k - \omega$ SST closure. As shown in Figure 2.1, the structured mesh is also refined near the vicinity of the throat in order to better capture the compressible phenomena. As the simulation is 2D, a total of 163 304 quadrilateral elements is used

2 | A HRM in density-based formulation

for each of the three geometries and the mesh independence is verified by comparing the simulation results of the regular mesh with the ones obtained using a mesh with twice as many elements in the axial direction. The two mesh grids were found to lead to indistinguishable results.

2.4 Results and discussion

In this section, the accuracy of the tabulated EoS is verified and discussed, also with regards to the metastable properties that require special treatment. The simulation speed is compared to a previous algorithm and the solver is validated in HEM against nozzle pressure profiles. Lastly, the HRM and HEM results are compared and the phenomenology of mass flow rate increase in HRM is explained.

2.4.1 Tabulated thermodynamic relations

The most influential thermodynamic relations required by the solver are those to find the pressure and the temperature as a function of ρ and e , in order to close the system of PDEs. Therefore, one focuses, in this section, on the tables generated for those quantities for analysis and validation purposes. Figure 2.6 displays the grids generated for pressure and temperature in the $(\rho - e)$ state space. The mesh for the pressure table was generated by imposing a maximum interpolation error of 0.1 [Pa] with relaxation to 0.1 [kPa] if the cell width (abscissa) is below 0.5 [kg/m³]. Note that only the validity region was represented in the figure so that the region in white is outside of said validity region. The generated grid is composed of 175 637 cells/sub-cells elements and requires roughly 35 MB of RAM during the CFD simulation. One can notice that, as expected, the majority of the elements are present along the saturation curve. Additional refinement can also be noticed in the near vicinity of the critical point in the center of the domain as the pressure gradients with respect to ρ and e are high in that region. In addition, the pressure grid requires more elements in the region of low energy and high density. Indeed, in this region the fluid is in the liquid phase and the pressure varies quite strongly with both state variables. For the temperature table, the error tolerance is set to 0.0001 [K] with relaxation to 0.001 [K] with the same cell width threshold. Likewise, the grid is composed of 96 589 cells/sub-cells elements and requires roughly 20 MB of RAM during the CFD simulation. As mentioned in Section 2.3.4, the tabulation algorithm contains some fallback mechanisms in order to

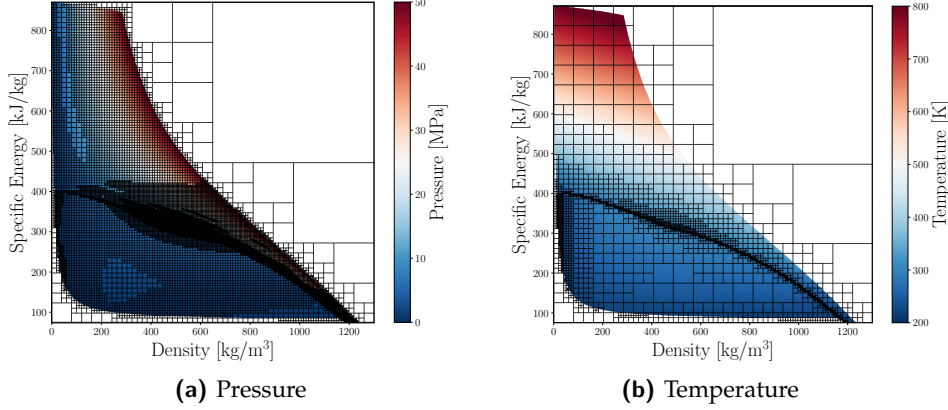


Fig. 2.6 Properties in the $\rho - e$ state space and mesh generated by the tabulation algorithm. The imposed precision for the tables is 0.1 [Pa] for pressure and 0.0001 [K] for temperature.

prevent non-physical values or excessive refinement. This is why it is important to verify the interpolation error a posteriori. Figure 2.7 displays the relative error, defined as:

$$\text{Relative Error} = \left| \frac{\chi_{\text{interp}} - \chi_{\text{sol}}}{\chi_{\text{sol}}} \right|, \quad (2.12)$$

for pressure and temperature. The plots were generated by taking 10^6 linearly spaced points in the $\rho - e$ state space. Again, only the validity range of the lookup table is shown. The relative error is mostly within the range $10^{-5} - 10^{-9}$ for the pressure. Actually, the higher errors, of the order of 10^{-3} are located in the very near vicinity of the saturation line. In practice, it is unlikely that the solution will contain a lower precision point, adding to the fact that said point still has a quite acceptable precision and won't prevent the solution from converging. Interestingly, some peculiar patterns can be observed in Figure 2.7. Those are naturally occurring within each generated cell and are an image of the curvature of the bi-cubic interpolation function within that cell. Indeed, upon close attention, one can notice that the error tends towards zero at the location of the interpolation points (Fig. 2.4), where the error is by construction zero and curves around in between. For HRM simulations, special care should be taken to compute the metastable properties. As per Figure 2.2, the metastable properties required

2 | A HRM in density-based formulation

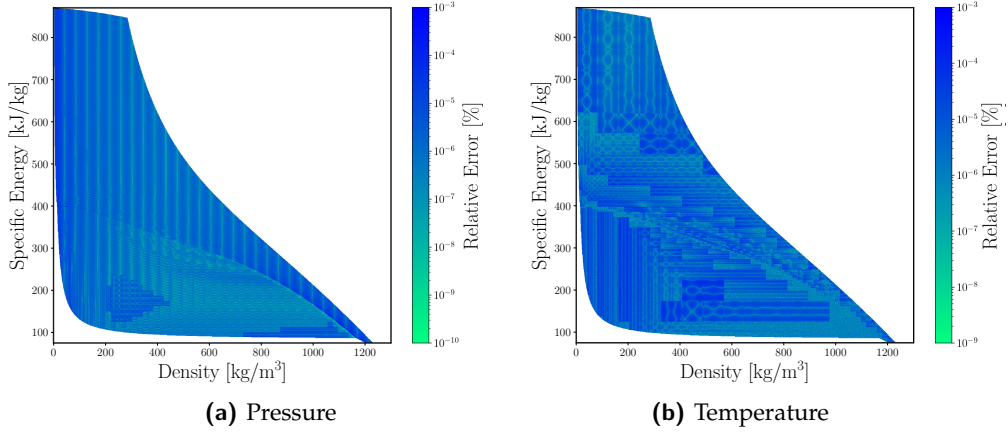


Fig. 2.7 Relatives errors in the $\rho - e$ state space.

for the algorithm are $\rho_{ml}(p, e_{ml})$ and $T_{ml}(p, e_{ml})$. Metastable properties (obtained from the REFPROP library) can be calculated in the portion of the thermodynamic state space comprised between the saturation curve and the *spinodal* limit, which is the limit beyond which a state becomes unstable. The

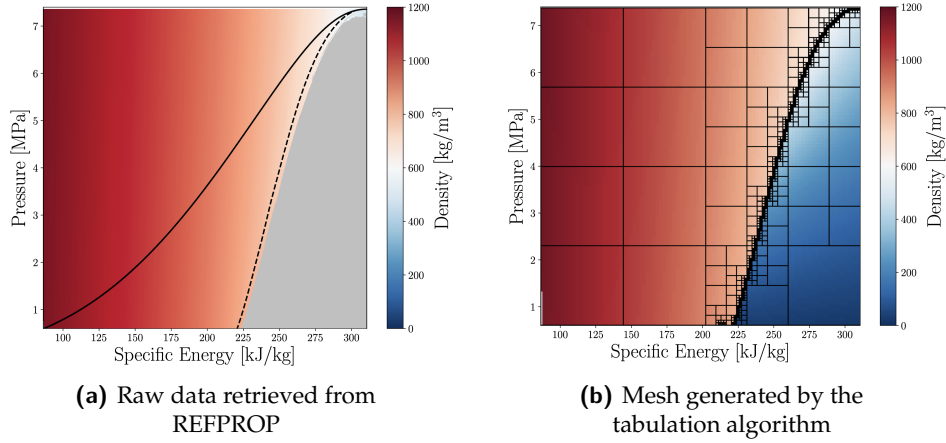


Fig. 2.8 Density in the $\rho - e$ state space including the metastable region. In Figure 2.8a, the invalid states are represented in gray, and the saturation curve (plain curve) and the approximated spinodal limit (dashed curve) are plotted.

spinodal limit can be expressed as the locus of thermodynamic states such that $\left. \frac{\partial p}{\partial v} \right|_T = 0$. Figure 2.8a shows the raw metastable density retrieved from the library, with the gray region indicating failure to compute said property. The spinodal limit is then the limit of the predictable region (that is, the limit between colored and gray regions). Because the spinodal is not sharply defined, especially near the critical point (Fig. 2.8a), it is reconstructed (with a safety margin in the abscissa direction) by a spline function. The invalid (grayed) region is then set to the equilibrium value to construct the interpolation table, as seen in Figure 2.8b. In practice (and for the results presented here), the properties are never retrieved from the reconstructed invalid region. Note also that only the left part (on the liquid side) of the spinodal limit has been considered, as the HRM is used to model *flashing* expansion processes only.

2.4.2 Table speed-up

To assess the performance of the novel tabulated method, the latter is compared to the tabulated method of [56] for the test case of Nakagawa *et al.* [117] (case c, Tab. 2.1). Figure 2.9 shows the speed-up, defined as $t_{(1 \text{ proc})} / t_{(n \text{ procs})}$, as well as the average iteration time as a function of the number of processors for both tables. Each simulation ran for 1000 iterations (on the converged solution) on the same cluster and the pre-processing time

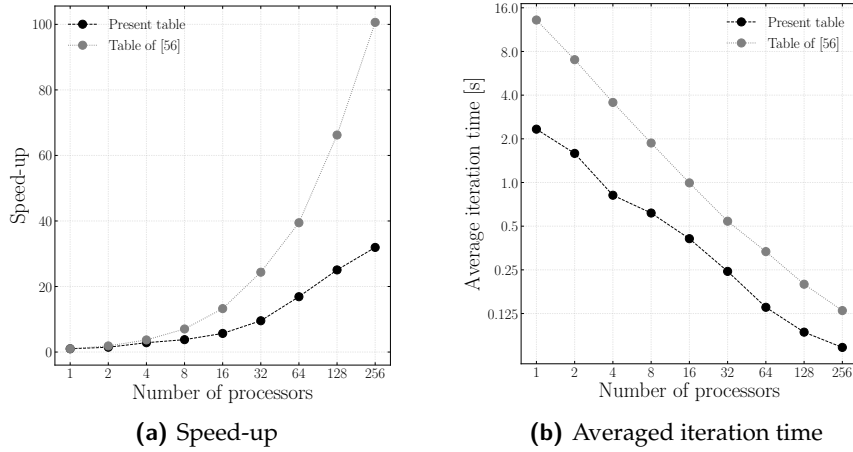


Fig. 2.9 Performance comparison between the present tabulated method and the one of [56].

was not taken into account. The speed-up increases more rapidly when using the table of [56], while the average iteration time is lower when using the present table (depending on conditions and number of CPUs, the present table is between 2 to 6 times faster). This indicates that the present tabulation method is indeed faster than the table of [56] but that there is less computation time gain obtained from the parallelization process (which is also a confirmation of the efficiency of the current approach). Note that despite the tabulated method of [56] being reported to perform roughly 66 times faster than the original Span-Wagner EoS for transcritical CO₂ applications, the tabulated equation of state constitutes the bottleneck in terms of simulation speed. The interested reader is invited to review the original article of [56] for a thorough description of the algorithm. If the calculation time required by the EoS is reduced, the time gain obtained / obtainable is reduced as well (since the present algorithm performs faster, other parts of the code, not related to the EoS, may limit the speed-up). In practice, this means that adding more CPUs while using the table of [56] will tend to compensate the low speed of the tabulated method, but it is not practical due to the finite amount of computational resources that is at disposition. Instead, the same simulations can be ran using significantly less resources with the present table.

2.4.3 Validation and verification of the solver

As demonstrated by Palacz *et al.* [122] in the context of ejector flows, the validity of the HEM decreases as the expansion occurs at lower temperatures. In addition, it can be expected that the metastable liquid phase should be more present at lower nozzle pressures since the metastable properties range is larger at lower pressures (Fig. 2.8). Therefore, it was chosen in the present work to study the nozzle expansion at temperatures below critical (Tab. 2.1) from the experiments of [117]. Figure 2.10 displays the comparison of the present CFD-HEM results with the experimental measurements. Note that two separate methods were used to measure the pressure: (i) by measuring the wall temperature and deducing the pressure from saturation properties ($p_{sat}(T)$); (ii) by direct pressure measurement with strain gauge (p_{strain}). As reported in [117], small holes were drilled along the centerline of both nozzle side walls, with eleven holes on one side for thermocouple taps and four holes on the other side for the strain-gauge taps. Static temperatures and pressures were simultaneously measured through the taps. Measurements were performed when steady state was reached, which was

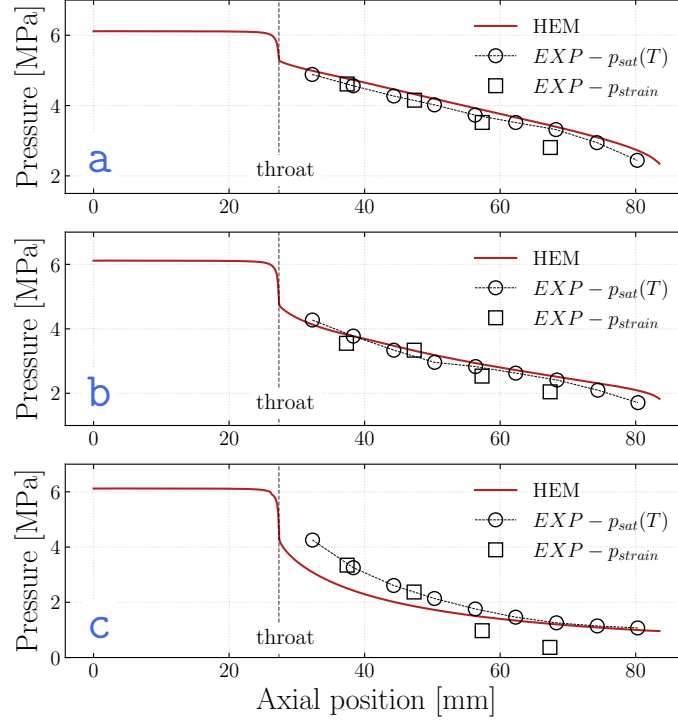


Fig. 2.10 Pressure profiles along the center-line of the nozzle (CFD) and comparison with the experimental data of Nakagawa *et al.* [117]. Please refer to Table 2.1 for geometrical and inlet parameters of cases a, b and c.

determined based on the profiles of the experimental run. The interested reader is invited to review the original paper of Nakagawa *et al.* [117] for detailed information about the experimental setup. Note that discrepancies between the two types of measurements may come from metastability effects, though it is the authors' understanding that the HRM might not be able to model those specific effects since, as discussed in Section 2.3.5, equilibrium conditions are expected at the wall. The measurements are then compared to the pressure at the center line of the nozzle, obtained from the converged HEM solution. Since the equilibrium is assumed (with HEM), there is no difference between the pressure field and the saturation pressure obtained from the temperature field ($p_{sat}(T)$). As seen in Figure 2.10, the prediction of the HEM is fairly accurate for cases a and b. For case c,

2 | A HRM in density-based formulation

discrepancies between the HEM and the experimental data are most visible in the first portion of the diffuser, where the simulation under-predicts the pressure. It was thus chosen to use case c to conduct the study on HRM and investigate the potential improvement of said model.

2.4.4 Homogeneous equilibrium vs homogeneous relaxation

As stated, the study presented in this section is conducted on case c (Tab. 2.1). Note also that as in the experiments of [117], the nozzle is fully choked. A parametric study is conducted to quantify and qualify the influence of the relaxation time on the local flow features as well as the mass flow rate within the nozzle. To this end, the results of the HEM simulation are compared to those of the HRM simulations performed with (i) three increasing relaxation times and (ii) the correlation of [8]. Note again that other correlations exist for CO₂ in the literature such as in the works of Haida *et al.* [70] or Log *et al.* [98], but those correlations have been found to yield relaxation times so high that the solution for the metastable properties is located in the unstable region for the investigated case: this also illustrates the lack of universality of such correlations. To the best of the authors' understanding, the value/correlation of θ is highly case-dependent and only the correlation of [8] was calibrated on the cases of Nakagawa *et al.* [117], though on higher inlet pressure cases of 9.1 [MPa] and never tested on the cases presented in the present work.

Pressure and quality profiles

One can first observe the behavior of the pressure curves along the nozzle axis as the relaxation time is varied, as shown in Figure 2.11. It is seen that consistent variation of θ leads to consistent modification of the pressure profile, that is, as the relaxation time is increased by steps of $5 \cdot 10^{-6}$ [s], the pressure profile in the divergent (where the flow is two phase) is lifted by similar increments. Interestingly, it appears that a constant value of $\theta = 15 \cdot 10^{-6}$ [s] fits best the first half of the divergent, but leads to an over-prediction in the second half, whereas the curve for $\theta = 5 \cdot 10^{-6}$ [s] fits best the second portion of the divergent. One could then argue that varying θ from $15 \cdot 10^{-6}$ [s] to $5 \cdot 10^{-6}$ [s] along the expansion could yield an optimal fitting. However, the raised pressure profile is a consequence of the physics that takes place in the near vicinity of the throat, where the metastability effects are most prominent and the relative difference of quality between HEM and HRM is most pronounced. In the second half of the divergent, the HEM and HRM pressures are actually very close to each

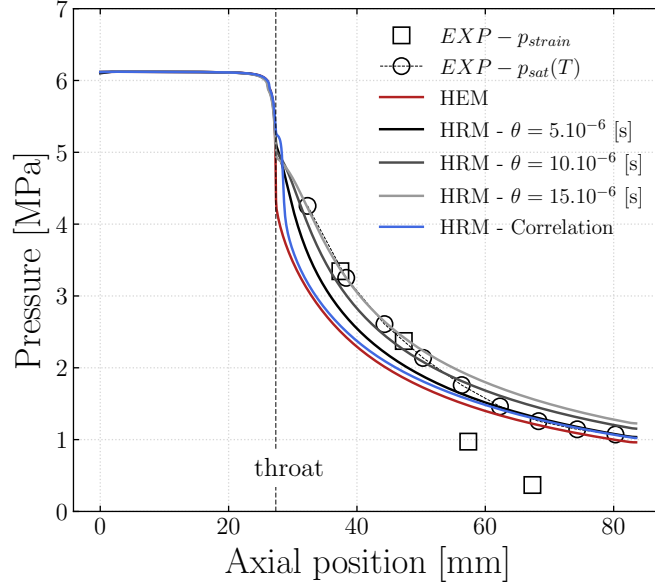


Fig. 2.11 Pressure profiles obtained for case c using HEM and HRM with different constant relaxation times and the correlation of [7], and comparison with experimental measurements [117].

other as the variation of the quality is low in that region. Thus, lowering θ along the divergent could not allow to recover a better fitting. In addition, one can see that the correlation of [8] yields little difference with the HEM solution and is not able to properly fit the experimental measurement. In fact, the relaxation time drops to extremely small values as the pressure gets lower (Eq. (2.6)) right after the throat location, which effectively creates a pressure shift in that very small region. Note at this stage it is possible that the measurements in the work of [117] could have some flaws. Indeed, as $p_{sat}(T) \approx p_{strain}$ in the first part of the diffuser, the flow should be at equilibrium from the experimental point of view. However, in this area, the pressure values clearly agree with the HRM with a large relaxation time, i.e., with a significant non-equilibrium. Inversely, there is a difference in the measured pressures according to the two different methods in the second half of the diffuser, meaning that a growing non-equilibrium appears in this part. Nevertheless, the profile of $p_{sat}(T)$ agrees well with the HEM and it is also expected, from a physical point of view, that the non-equilibrium tends to damp out along the pipe as HEM and HRM predictions become closer.

2 | A HRM in density-based formulation

In addition, the present analysis, using the HRM, also indicates that the flow is at equilibrium at the wall (i.e., where the measurements are taken). This is verified in Figure 2.12 by analyzing the relative difference of quality with respect to the equilibrium ($(x_{eq} - x)/x_{eq}$) and the pressure profiles obtained from the pressure field p directly and via the temperature field ($p_{sat}(T)$). The profiles are plotted at the wall as well as at the center line for reference, and for two different values of the relaxation time. As one can see, the difference between quality and equilibrium quality is negligible at the wall, and the pressures profiles obtained using both methods are equal, indicating that the fluid is indeed at equilibrium at the wall. Moreover, one can see when comparing Figures 2.12a and 2.12b that as θ is increased, the difference between p_{center} and $p_{sat}(T_{center})$ increases as well, whereas the wall seems to remain at equilibrium pressure. Likewise, with a higher θ , the relative difference of qualities in the centerline gets higher and extends further into the divergent, but seems to remain somewhat negligible at the wall. Note also that the pressure appears to be uniform at a given axial position. As stated in Section 2.4.3, the experimental measurements are done on the side walls, at the center line, and not at the upper/lower walls. Nonetheless, it is still expected, by the same logic, that the fluid will be at equilibrium at the side walls. This further encourages the authors to believe that the experimental pressure measurement should not be used to quantify the actual degree of non-equilibrium. The size of the holes to connect the

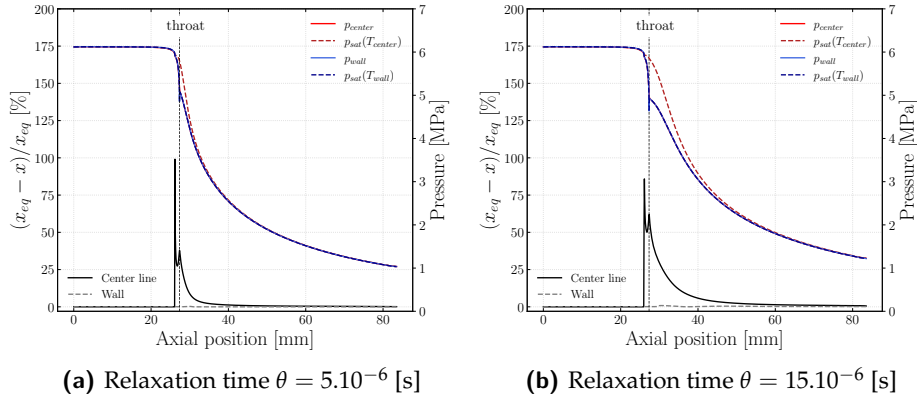


Fig. 2.12 Relative difference of quality with respect to the equilibrium and pressure profiles using different methods at the center line and at the wall for case c.

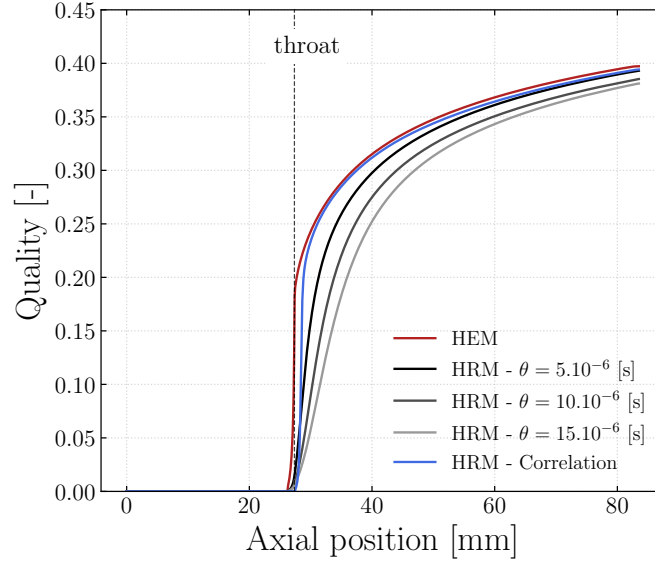


Fig. 2.13 Quality profiles obtained for case c using HEM and HRM with different constant relaxation times and the correlation of [7].

pressure taps compared to the very small dimensions of the part (0.24 [mm] at the throat) is not provided, and possible heat transfer features are not discussed for the measurements of $p_{sat}(T)$ in [117].

Figure 2.13 presents quality profiles along the center line of the nozzle. The effect of the relaxation time can there be seen, as it delays flashing by reducing the slope of the quality profile.

Local flow features and mass flow rates

In this section, the local flow fields of velocity (Fig. 2.14) and density (Fig. 2.15) are compared, which allows to describe the mechanism leading to the increase of the mass flow rate in HRM, that is associated to two competing phenomena. On one hand, as seen in Figure 2.14, increasing the relaxation time reduces the velocity in the divergent, which tends to decrease the mass flow rate. On the other hand, as shown in Figure 2.15, increasing θ also results in the increase of the density, which increases the mass flow rate. Note that those observations are consistent with the ones obtained by Palacz et al. [121] using their pressure-based solver to perform HRM simulations of ejectors. The competition of those two mechanisms, in the end, result in the increase of the mass flow rate with θ as the density effect is dominating.

2 | A HRM in density-based formulation

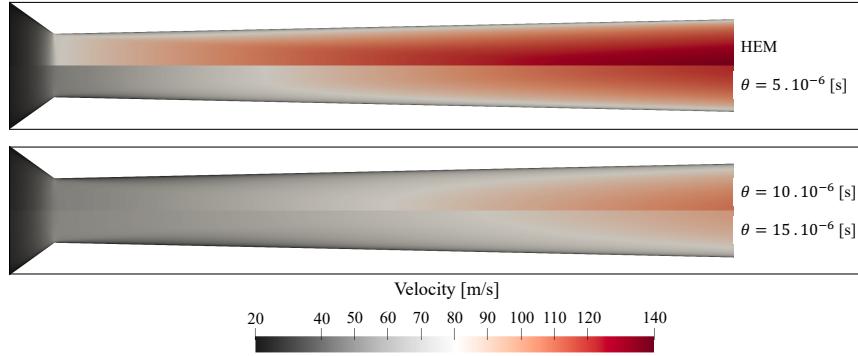


Fig. 2.14 Fields of the mean axial velocity component obtained for case c using HEM and HRM with different relaxation times. The geometry was stretched X4 in the vertical direction for better readability.

Table 2.2 summarizes the mass flow rate effects of the relaxation time for each case. The mass flow rate increase obtained with θ grows quickly to non-negligible values. In the case that fits best the pressure profile in the first portion of the diffuser (Fig. 2.11), i.e., $\theta = 15 \cdot 10^{-6}$ [s], the mass flow rate is increased by more than 18%. Although no mass flow measurements were performed in the experiment [117], one can appreciate metastability effects. As explained in [40], introducing instabilities generally leads to an increase in the speed of sound, which can increase the mass flow rate under

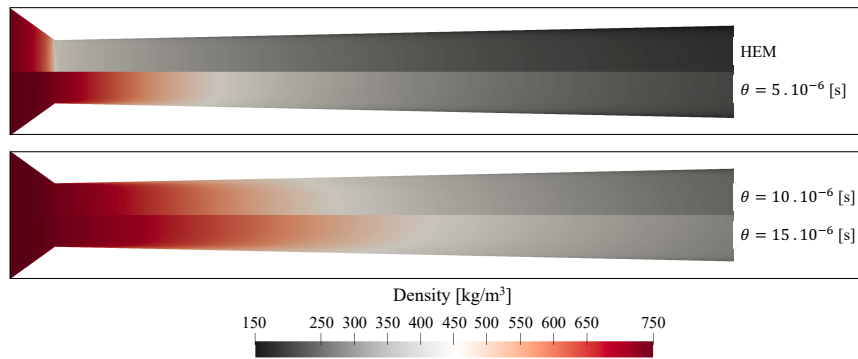


Fig. 2.15 Density fields obtained for case c using HEM and HRM with different relaxation times. The geometry was stretched X4 in the vertical direction for better readability.

	Mass flow rate [g/s]	Increase w.r.t. HEM [%]
HEM	23.07	/
HRM - $\theta = 5.10^{-6}$ [s]	24.69	7.02
HRM - $\theta = 10.10^{-6}$ [s]	26.16	13.40
HRM - $\theta = 15.10^{-6}$ [s]	27.30	18.34
HRM - Correlation of [8]	23.19	0.52

Table 2.2 Mass flow rate and increase with respect to the HEM solution for case c with various relaxation times and the correlation of [8].

choked conditions and modify the pressure profiles. However, as numerical models such as the present one do not include the whole flow physics and non-equilibria, discrepancies between numerical results and experimental measurements may be still expected.

2.5 Conclusions

In this work, two advances were made towards wall-resolved simulations of flashing CO₂ nozzles and ejectors. Firstly, a novel general method for the construction and interpolation of the equation of state was described. The method is based on bi-cubic functions and a quad-tree algorithm with local refinement of the interpolation grid in the thermodynamic state-space. It was found that this method allows for both reasonable storage size of the tabulated properties and fast interpolation speed during the CFD simulations. Although the method is here used in the context of CO₂ only, it can be applied without modification to generate any table linking three thermodynamic properties for any fluid, given that the relation is obtainable from an external source (as in the present case, through the REFPROP and COOLPROP libraries). The table generation method is based on a provided absolute error tolerance, and it was verified a posteriori that the interpolation error is indeed below the required threshold.

Secondly, a density-based formulation of the HRM was implemented for the first time in a CFD frame and the impact of the relaxation time was studied by employing both constant values and the correlation of Angielczyk et al. [8] that was calibrated on similar flashing CO₂ nozzle cases. The pressure and quality profiles within the device were found to behave in a consistent manner, also in agreement with regards to the current literature. It was observed that as a constant relaxation time was increased, the pressure

profiles in the fully supersonic nozzle were shifted upward and the jump in the quality profiles was smoothed, inducing a delay in the flashing process. In addition, the mass flow rates increased significantly, accounting for more than 18 % when the pressure profile is best fitted by the HRM in the near-throat region. It was also found that the best fit with constant relaxation time in the first half of the diffuser over-predicted the pressure in the second half, and that a lower relaxation time was best in that region.

Nonetheless, the study indicates that the metastability effects in HRM are mostly occurring in the near vicinity of the throat (i.e., where flashing occurs), and therefore the worse pressure fitting in the second half of the diffuser was essentially a consequence of the delay in the first half of the diffuser. This is confirmed by the results obtained with the correlation of Angielczyk *et al.* [8] for the relaxation time, where the latter takes non-negligible values only in a very small region near the throat, leading nonetheless to a similar rise of the pressure profile downstream. Said correlation yielded poor results with no significant mass flow rate increase, which may indicate that the required value of the relaxation time is highly case dependent and that it is unlikely that one may find a universal law for the current HRM framework. Furthermore, it is the understanding of the authors that only a correlation including negative relaxation times would allow pressure fitting along the entirety of the nozzle, where one would have positive (physical) relaxation times in the first portion of the diffuser, decreasing to reach negative (non-physical) values downstream to counteract the pressure rise induced upstream. This may indicate that some physics is missing in the HRM. Therefore, it could be interesting, in future works, to re-introduce the saturated-liquid phase lacking in the current HRM framework to develop a new hybrid model. Lastly, one may point out the crucial lack of quality experimental measurements (pressure and temperature profiles, mass flow rates) that are needed in order to fully understand what phenomena are at play within flashing CO₂ nozzles and ejectors.

3

Theoretical Analysis of the Optimal Ejector Operation and Design Within an Ejector-Based Refrigeration System

3.1 Foreword

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Abstract:

Optimal operation and design of ejectors are the subject of recent concerns, especially for the enhancement of refrigeration and heat pump cycles based on natural refrigerants like carbon dioxide. In this study, a thermodynamic analysis of an ejector-based refrigeration cycle is performed to determine both what operating pressures lead to the highest physically possible performance depending on the ambient conditions, and what are the main dimensions of the ejector leading to the best performance at a given ambient temperature. A state-of-the-art thermodynamic model for the prediction of the ejector performance is for the first time utilized to generate reliable operation and performance maps of the ejector cycle. Most notably, it is found that the optimal coefficient of performance is not necessarily found when the ejector operates at critical conditions but mostly when the device is under off-design regime, depending on the ejector internal efficiency and the gas cooler outlet temperature. In addition, the analysis reveals that the performance of the cycle is not highly sensitive to the throat area ratio of the ejector given that the latter lies within an acceptable range. Those findings contribute to getting a better understanding of how the cycle benefits from the ejector and define design and control strategies for the cycle.

3.2 Introduction

Ejector refrigeration systems (ERSs) are becoming a compelling alternative to the classical refrigeration cycle since these systems can recover part of the exergy losses that occur at the expansion level. Originally motivated by the transition towards natural refrigerants that tend to have lesser performances than fluorocarbons (CFCs, HCFCs and HFCs), the integration and optimal operation of the ejector within the refrigeration system are now the subject of many works (see in [17]). Carbon dioxide (CO₂) has emerged as an appealing choice for a working fluid due to its non-toxic and non-flammable properties. Additionally, the shift towards CO₂ utilization has been driven by international agreements like the Kyoto Protocol, which

mandates phased reductions in the use of HCFCs and HFCs within the next two decades [2]. In Europe, the revised F-gas regulation aims at reducing the EU's fluorinated greenhouse gas emissions by two-thirds by 2030.

Because carbon dioxide has a critical temperature of 31 [°C], the cycle must often operate under *transcritical* conditions depending on the ambient temperature. However, operating at higher temperatures requires high compression of the refrigerant, which quickly introduces notable losses in the expansion valve due to the high pressure ratio [79] and the higher entropy production of CO₂ during the isenthalpic expansion compared to classical refrigerants [52]. The design of CO₂ ejectors and the optimal operation of the CO₂ ERS are therefore subject of recent concerns for the enhancement of the performance of the refrigeration systems [15]. Yet, ejectors are known to have intricate fluid dynamics, and it is the authors' opinion that certain underlying mechanisms within these devices (e.g., the double choking mechanism) remain not fully understood and often poorly modeled, which may lead to sub-optimal ejector design and contributes to hamper operation strategies of the ERS.

In 1931, Gay [62] first proposed the basic transcritical CO₂ ejector refrigeration system (as shown in Figure 3.1, Section 3.3.1). This configuration has since been demonstrated to yield the highest coefficient of performance (COP) and exergy efficiency among the proposed layouts for CO₂ systems [142]. The high pressure supercritical CO₂ coming from the gas cooler is expanded in the ejector, thereby pre-compressing the gas CO₂ coming from the evaporator, and the refrigerant thus has an intermediate pressure at the compressor inlet, so that the compressor can operate at a lower charge. In addition, the ejector can improve the evaporator performance due to the consequently near-liquid feeding operation [123]. In 1990, Kornhauser [80] performed a first analysis of cycle performance using a simple in-house ejector heat pump model that was implemented as a Fortran routine. The author [80] compared the performance of a standard vapor compression cycle and an ERS for different refrigerants and found potential COP improvements ranging from 12% to 30%. Nehdi et al. [118] later developed a computer code that uses fluid properties retrieved from NIST REFPROP to evaluate the influence of the ejector area ratios on the cycle performance. The analysis was performed for several refrigerants and it was concluded that a maximum COP improvement of 22% could be achieved by using an ejector in R141b systems, which was the most favorable case. Bilir Sag et al. [19] used a similar routine to investigate the two-phase R134a ERS and found a similar range of potential COP improvement. In addition, the

authors [19] noted that even if the ejector worked under off-design regime, the cycle performance still benefited from the ejector. Several similar studies have been subsequently performed to investigate the influence of the ejector on the cycle performance [78, 88, 133, 152].

In 2005, Li and Groll [87] studied the influence of operating parameters on the COP of the CO₂ cycle. Most notably, the authors found that the COP of the ERS could be improved by more than 16% over the basic transcritical cycle, for typical air conditioning operating conditions. Several theoretical works have later been done to assess the performance of the CO₂ ERS specifically [44, 58, 81, 151, 153]. Notably, Fangtian and Yitai [58] performed an exergy analysis to evaluate the losses in the different parts of the cycle and found that there exists a critical entrainment ratio, a critical gas cooler outlet temperature and an optimal heat rejection pressure that optimize the cycle operation. Some studies then focused on modifying the geometry of the ejector itself to be able to match the optimal operating conditions as closely as possible. Elbel and Hrnjak [51] found out that regulating the high-side pressure with an ejector needle could be a way of optimizing the cycle performance, much as for a traditional expansion valve cycle. Alternatively, multi-ejector systems received growing interest in the recent years and are already commercialized in the form of ejector packs that comprise cartridges containing several ejectors of different sizes and internal geometries. Depending on the operating conditions, some ejectors are then activated through the action of solenoid valves [10, 138].

Some recent studies [32, 92, 93, 96] have also opted to use the Dymola commercial software, that allows to perform transient operation analyses with out-of-the-box components models available in commercial libraries. Recently, Metsue *et al.* [109] investigated the influence of the ejector geometry on the performance of a transcritical CO₂ ejector cycle using Dymola. The authors used their in-house ejector model [110] calibrated onto the CO₂ experimental data of Zhu *et al.* [155] and found that there exists an ejector size that maximizes the COP of the cycle, and that critical ejector pressure is not reached at this optimum COP point. Rather, the ejector is operating well under the on-design regime.

Nonetheless, the authors believe that a deep understanding of the link between ejector operating regime and overall cycle performance is still lacking. Yet, this knowledge is fundamental to set up efficient design strategies at the component level and determine adequate cycle operation strategies. In this study, the classical CO₂ ERS is analyzed theoretically to give insight onto the optimal operation pressures of the cycle. To this end, a typical

refrigeration application (e.g., air conditioning) is considered. The operation of the ejector is predicted using the state-of-the-art ejector thermodynamic model of Metsue et al. [110], that integrates the natural physics of the compound-choking theory for predicting double-choking operation. This allows to establish the domain of operation that is allowable by the physics and determine the operating pressures that yield the highest coefficient of performance. A parametric analysis of the secondary to primary throat area ratio of the device is also carried out to find the optimal ejector dimensions for specific operation temperatures and determine the sensitivity of the COP to this geometrical parameter. The link between the cycle performance and the operating regime of the ejector is investigated, and the effects of the entropy-generating mixing phenomena within the device are highlighted.

3.3 Thermodynamic modeling

The numerical modeling of the ejector cycle is here described. In Section 3.3.1, the system is first solved assuming an ejector that can provide any performance required by the cycle. In Section 3.3.2, the ejector entrainment ratio is then calculated with the real ejector thermodynamic model to determine the actual possible operation of the device (i.e., that could also be allowed to fulfill the physical conditions).

3.3.1 Cycle modeling

As stated in the previous section, the present work focuses on the analysis of the classical refrigeration cycle shown in Figure 3.1. The system is modeled with the following assumptions:

- The cycle operates in steady state.
- The ambient temperature T_{amb} (external) is fixed. Three values of T_{amb} will be considered in the following: 15, 25 and 35 [°C].
- The cooling temperature (external) is fixed to $T_{cool} = 4$ [°C].
- The pinch temperatures at the gas cooler $\Delta T_{pinch, gc} = T_3 - T_{amb}$ and at the evaporator $\Delta T_{pinch, ev} = T_{cool} - T_{10}$ are both assumed to be of 10 [°C] (typically the pinch temperature ranges between 5 and 10 [°C] [38]).
- There are no pressure drops across the gas cooler and the evaporator.

3 | Performance analysis of the ERS

- The refrigerant is at saturated vapor state at the evaporator outlet.
- The thermodynamic transformations within the ejector, expansion valve and separator are adiabatic.
- The thermodynamic transformation within the compressor is isentropic. Note that this hypothesis is not true in practice, but this does not constitute the subject of the present analysis for which a simple transformation is sufficient.

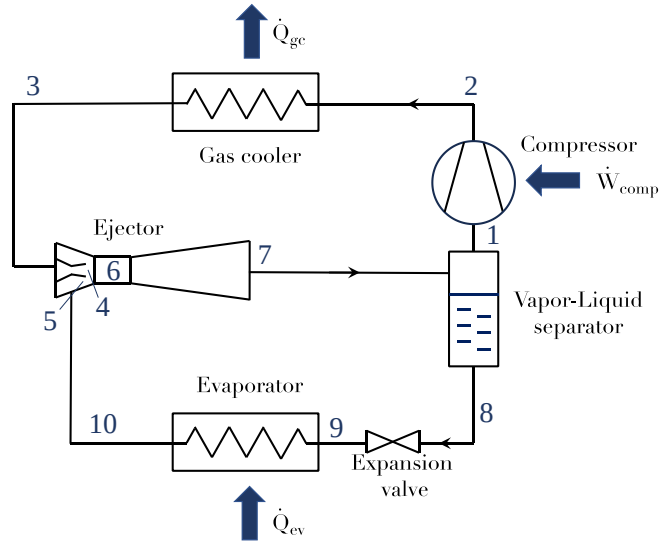


Fig. 3.1 Classical ejector refrigeration system. The main locations of the cycle have been numbered for reference within the text.

Note that the pressure at the gas cooler p_{gc} and at the outlet of the ejector p_{out} are not constrained and those have thus to be imposed in order to solve the system. Based on those hypotheses, the global energy conservation of the system can be expressed as:

$$\dot{Q}_{ev} + \dot{W}_{comp} + \dot{Q}_{gc} = 0, \quad (3.1)$$

where $\dot{Q}_{ev}$ is the cooling power accumulated by the evaporator, $\dot{W}_{comp}$ is the compression mechanical power and $\dot{Q}_{gc}$ is the heat power discharged at the gas cooler. Also note that in this work the energy introduced into the

system is chosen to be positive by convention. From the aforementioned assumptions, Eq. (3.1) can then be re-written in terms of specific enthalpies:

$$\dot{m}_s(h_{10} - h_9) + \dot{m}_p(h_2 - h_1) + \dot{m}_p(h_3 - h_2) = 0, \quad (3.2)$$

with $\dot{m}_p$ and $\dot{m}_s$ the primary and secondary mass flow rates, respectively. The number indices on the enthalpy terms (h_i) refer to their position in the cycle (Fig. 3.1). When dealing with ejectors, an important quantity to monitor is the secondary to primary flow ratio, which is referred to as the entrainment ratio, as the –secondary– flow coming from the evaporator is entrained by the discharged –primary– flow that comes from the gas cooler. The entrainment ratio $\omega = \dot{m}_s / \dot{m}_p$ can then be deduced from Eq. (3.2):

$$\omega = \frac{h_1 - h_3}{h_{10} - h_8}, \quad (3.3)$$

where the enthalpy conservation across the expansion valve was used, i.e., $h_9 = h_8$. A similar expression can be found for the COP, for which the general expression, for a cooling cycle, is given by [118]:

$$COP = \frac{\dot{Q}_{ev}}{\dot{W}_{comp}}. \quad (3.4)$$

Much as for ω , the COP can be expressed as a function of the enthalpies:

$$COP = \frac{\dot{m}_s}{\dot{m}_p} \frac{h_{10} - h_9}{h_2 - h_1} = \omega \frac{h_{10} - h_9}{h_2 - h_1} = \frac{h_1 - h_3}{h_2 - h_1}. \quad (3.5)$$

The cycle can then be fully solved on the basis of the previous assumptions, and the mass conservation equation of the liquid phase at the separator, i.e.:

$$\dot{m}_s = (\dot{m}_p + \dot{m}_s)(1 - x_7), \quad (3.6)$$

with x the vapor quality. The quality at the inlet of the separator can therefore be expressed as a function of the entrainment ratio only:

$$x_7 = \frac{\dot{m}_p}{\dot{m}_p + \dot{m}_s} = \frac{1}{1 + \omega}. \quad (3.7)$$

As it is well known, the thermodynamic state of the working fluid is determined by two independent state variables (pressure and temperature

3 | Performance analysis of the ERS

Point	State variable 1	State variable 2
1	$p_1 = p_{out}$	$x_1 = 1$
2	$p_2 = p_{gc}$	$s_2 = s_1$
3	$p_3 = p_{gc}$	$T_3 = T_{amb} + T_{pinch, gc}$
7	$p_7 = p_{out}$	$x_7 = 1/(1 + \omega)$
8	$p_8 = p_{out}$	$x_8 = 0$
9	$p_9 = p_{10}$	$h_9 = h_8$
10	$T_{10} = T_{cool} - T_{pinch, ev}$	$x_{10} = 1$

Table 3.1 Pair of state variables to solve the cycle at each relevant point.

are not independent under the saturation dome). To this end, Table 3.1 summarizes the pair of state variables that are used at each relevant point of the cycle. Then, all other state variables can be retrieved from the equation of state. In the present work, the latter is provided by the COOLPROP library [13]. The cycle can then be represented in the $p - h$ diagram, as shown in Figure 3.2 for typical operation of the ERS. Note that points 4,

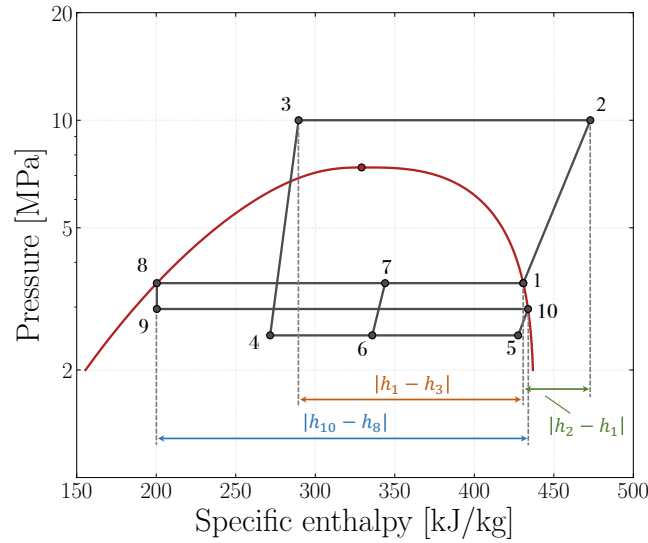


Fig. 3.2 Classical ERS represented in the $p - h$ diagram. Operating conditions are $p_{gc} = 100$ [bar], $p_{out} = 35$ [bar], $T_{amb} = 25$ [°C] and $T_{cool} = 4$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). Note that the y axis is in log scale.

5 and 6 are technically within the ejector and correspond to the primary stream at the primary nozzle outlet, secondary stream at the primary nozzle outlet and mixed flow at the secondary throat, respectively (Fig. 3.1). Figure 3.2 allows one to better visualize the enthalpy differences in the expressions of ω and COP in Eqs. (3.3) and (3.5), respectively: $\omega = (h_1 - h_3)/(h_{10} - h_8)$, $\text{COP} = (h_1 - h_3)/(h_2 - h_1)$.

It is important to mention at this stage that the value of ω predicted by Eq. (3.3) does not account for any internal mixing phenomenon. Rather, Eq. (3.3) constitutes the criterion for steady state operation of the cycle as it is derived from the global conservation of energy through the system. In other words, at each set of gas cooler and ejector outlet pressures, a specific value of the entrainment ratio is required by the cycle (determined by Eq. (3.3)). Therefore, this pseudo ejector model will be referred to as the cycle requirement model in what follows. In this manner, the cycle requirement model can predict the operation of the cycle for any set of operating pressure. Nonetheless, and as it will be seen in Section 3.4, only specific sets of operating pressures are allowed in an actual ejector cycle.

3.3.2 Ejector thermodynamic model

As stated previously, the thermodynamic model of Metsue et al. [110] is used to predict the performance of the real ejector (as opposed to the cycle requirement). This 0D model discretizes the ejector into several section, as seen in Figure 3.3, labeled from 0 to d , and the flow is solved at those discrete locations only. The choking of the device is modeled by the compound-choking theory [85, 110], which constitutes the natural condition for the choking of a multi-stream device such as the ejector, as it maximizes the total mass flow rate within the device. The model has already been validated for transcritical CO₂ applications by the authors in [109], where the

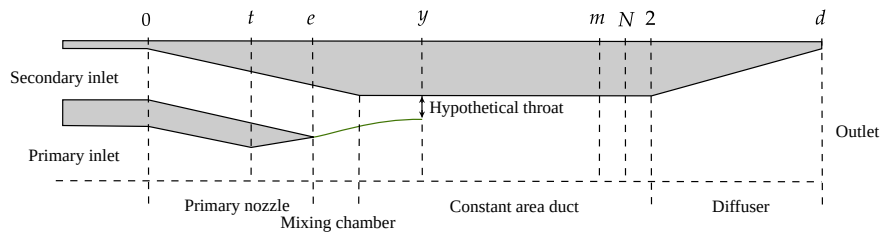


Fig. 3.3 Schematic of the ejector model, after Metsue et al. [110].

characteristic curves are calibrated on the experimental data of Zhu et al. [155]. The interested reader is invited to review the article of Metsue et al. [110] for a thorough description of the implementation/validation of the thermodynamic model, as only a brief summary of the model assumptions is presented in what follows. As explained in Metsue et al. [110], the flow within the system is considered to be one-dimensional, steady, and adiabatic, with negligible velocities at the inlets (primary/secondary) and outlet. To incorporate friction losses along the walls and within the shear layer between the primary and secondary streams, isentropic efficiencies are employed (Fig. 3.3). These efficiencies include η_p for the primary nozzle (between sections 0 and e), η_{py} for the friction losses encountered by the primary flow within the mixing chamber (between sections e and y), η_s for the friction losses experienced by the secondary flow within the mixing chamber (between sections 0 and y), and η_d for the diffuser (between sections 2 and d). Additionally, mixing losses between the primary and secondary streams are factored in through a loss coefficient η_m (between sections y and m). Furthermore, it is assumed that the primary and secondary streams remain distinct (i.e., no mixing) until they reach a specific section within the constant area duct. At this section, both pressures are considered to be equal, indicating the start of the mixing phenomenon. This section is often referred to as the hypothetical throat in the literature [72]. If the ejector operates under a double-choking regime, this section becomes compound-choked. The boundary between single- and double-choking operation of the ejector is then referred to as the critical operating condition or the critical point. In between each section of the model, the mass and total enthalpy conservation equations are applied. In addition, the equation of state provided by COOLPROP and the isentropic efficiency relations (for losses) are used. The momentum conservation equation is also used to handle the mixing, i.e., between sections y and m . In the present work, and as in [109], it is chosen to reduce the number of fitting coefficients since some of them have redundant effects on the predicted performance [110]. Therefore, it is chosen to set $\eta_{py} = \eta_s$ and $\eta_m = 1$, thus yielding the set of fitting efficiencies at ($\eta_p = 0.95$, $\eta_{py} = 0.73$, $\eta_s = 0.73$, $\eta_m = 1$, $\eta_d = 0.85$), which have been calibrated on the experimental data of Zhu et al. [155]. Figure 3.4 shows the result of the fitting of the ejector model on the experimental characteristic curves reported in [155] for transcritical operation. First, η_p is adjusted to fit the primary mass flow rate (the separate values for the primary and secondary mass flow rates are provided in [155]). Then, η_{py} and η_s are adjusted to match the entrainment ratio at on-design

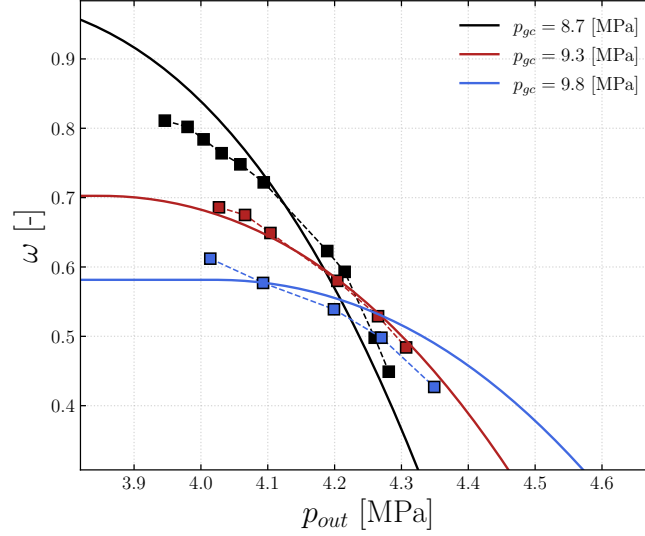


Fig. 3.4 Fitting of the ejector model onto the experimental data of Zhu et al. [155] ($\eta_p = 0.95$, $\eta_{py} = 0.73$, $\eta_s = 0.73$, $\eta_m = 1$, $\eta_d = 0.85$). The experimental data are shown with squares and the thermodynamic model predictions in plain lines.

operation, and the position of the off-design part of the characteristic curve is finally adjusted via η_d . In Figure 3.4, the efficiencies were tuned to obtain a good fitting for $p_{gc} = 9.3$ [MPa], and kept constant to generate the curves at $p_{gc} = 8.7$ and 9.8 [MPa], for which an acceptable fitting ability of the model is also observed. In the following, the efficiencies will thus be kept to those constant values. Note also that no cooling power is specified for the analysis, therefore the size of the component is not relevant and for the ejector, only the throat area ratio (TAR) A_y/A_t , with A the section area, is necessary to solve the system. To this end, a base TAR is chosen as the one of the ejector of Zhu et al. [155]: $A_y/A_t = 6.25$. This base TAR will be later optimized in Section 3.4.3. Moreover, the primary nozzle of the ejector of [155] is converging only, meaning that $A_e = A_t$. Nonetheless, the influence of A_e/A_t will be discussed in Section 3.4.3 as well.

3.4 Results and discussion

In this section, it is proposed to analyze the operation of the classical ERS by combining the approaches presented in Sections 3.3.1 and 3.3.2. This allows

3 | Performance analysis of the ERS

to both shed light onto the optimal and physically possible operating point of the cycle, as well as to determine what ejector TAR best suits the system, depending on the ambient temperature.

3.4.1 Entrainment ratio maps

As a first step, it is proposed to compare the entrainment ratios calculated using the two approaches, i.e., using the cycle requirement model (Section 3.3.1) and the real ejector model (Section 3.3.2). This is done by building maps of ω as a function of the pressure at the outlet of the ejector p_{out} and the pressure at the gas cooler p_{gc} . The maps boundaries for said pressures are set as follows:

$$\begin{aligned} p_{out} &\in [p_{10}, p_{crit}], \\ p_{gc} &\in [p_{down}, p_{up}], \end{aligned} \quad (3.8)$$

where the *crit* subscript refers to the critical conditions ($p_{crit} = 7.37$ [MPa]). The boundaries for p_{gc} (p_{down} and p_{up}) are free and are thus set as inputs. In the present work and without additional mention, the boundaries are set as ($p_{down} = 5.5$ [MPa], $p_{up} = 50$ [MPa]), which is deemed adequate for the present purpose. Figure 3.5 presents maps of the entrainment ratio using the cycle requirement model (Fig. 3.5a) and the real ejector model (Fig.

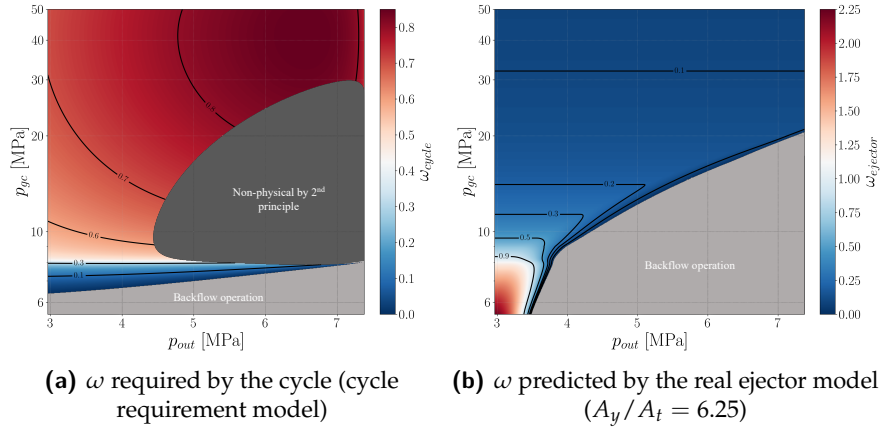


Fig. 3.5 Maps of the entrainment ratio ω as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} for $T_{amb} = 25$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). Iso- ω lines are plotted in black.

3.5b) for an ambient temperature of 25 [°C]. As it can be seen, additional portions of the maps have been discarded (in gray). The light gray regions indicate that the cycle was predicted to operate under backflow mode: under those conditions, the flow goes from point 10 to point 9 (Fig. 3.1). The dark gray region in Figure 3.5a indicates that the second principle of thermodynamics is not satisfied, i.e., $(\dot{m}_p + \dot{m}_s) s_7 < \dot{m}_p s_3 + \dot{m}_s s_{10}$. From Figure 3.5a, it appears that the entrainment ratio does not vary strongly with p_{out} for gas cooler pressures below 10 [MPa] (typical operation range of ERSs). On the other hand, at constant p_{gc} , the real ejector performance prediction (Fig. 3.5b) indicates a constant ω plateau and a rapid decline as the critical pressure of the ejector is exceeded. Actually, each line of the map (i.e., varying p_{out} at constant p_{gc} in Figure 3.5b) corresponds to an ejector characteristic curve (as described in [110]), since all inlet parameters are constant.

3.4.2 Operation of the ERS

To determine the actual –allowable– operation of the ERS, one must find the locus of operating pressures ($p_{gc} - p_{out}$) that satisfies the matching between the entrainment ratio required by the cycle (Fig. 3.5a) and that provided by the ejector (Fig. 3.5b). This said locus is referred to, in the present work, as the operation curve of the cycle. Practically, the operation curve is determined by calculating the entrainment ratio required by the cycle and that predicted by the real ejector model within the ($p_{gc} - p_{out}$) domain, as in Figure 3.5. Then, the difference in terms of entrainment ratio is computed at each point of the domain in order to find the zero, that corresponds, by definition, to the operation curve. Consequently, the operation curve is comprised of all sets of ($p_{gc} - p_{out}$) such that $\omega_{cycle} = \omega_{ejector}$. In this section, the operation curves are studied for three ambient temperatures (15, 25 and 35 [°C]). Note however that in the case of $T_{amb} = 15$ [°C], the cycle is not transcritical since the heat rejection (transformation 2 to 3, Fig. 3.2) at the hot side takes place at a pressure below the critical pressure. Figure 3.6 shows the COP map for the three selected ambient temperatures. The operation curves of the cycle using the ejector model calibrated on the experiment of [155] have been plotted in purple. The green curve corresponds to the operation curve of the cycle obtained by setting all efficiencies of the real ejector thermodynamic model to 1 ($\eta_i = 1$). The dots on the operation curves represent the point of maximum COP. The dotted lines represent the lines of critical operation of the ejector (obtained with the thermodynamic

3 | Performance analysis of the ERS

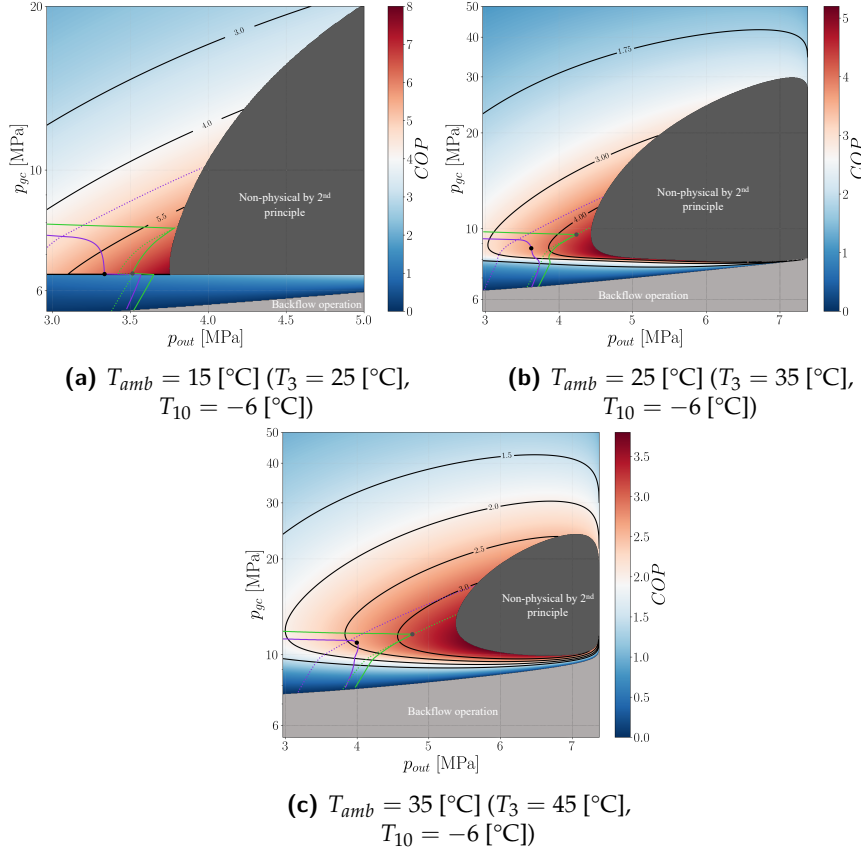


Fig. 3.6 Map of the COP as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} . The purple line is the operation curve with the fitting for the ejector of [155] and the green line the case with all $\eta_i = 1$. The on-/off-design limit is plotted in dotted lines and the maximum COPs are highlighted with dots.

model), separating the on-design regime (on the left) from the off-design regime (on the right). It can be seen that for the three ambient temperatures, the maximum COP point on the purple curve (ejector calibrated on [155]) is found when the ejector operates under off-design regime. This indicates that from the cycle's perspective, it is preferable to have a slightly higher outlet pressure (or equivalently, compression ratio p_7/p_{10}) even if it comes at the price of having a somewhat lower entrainment ratio (Fig. 3.5a). Notice also in Figure 3.6a that there appears to be a discontinuity at $p_{gc} = 6.43$

[MPa], which corresponds to the saturation pressure at the gas cooler outlet temperature $p_{sat}(T_3)$ (this case is subcritical, as mentioned previously). Thus, as T_3 is fixed, for $p_{gc} > 6.43$ [MPa], there is a condensation process (transformation 2 to 3 goes through the saturation dome), but for $p_{gc} < 6.43$ [MPa], there is no condensation of the hot refrigerant (point 3 is a gas), leading to the poor performance that may be noticed in that region in Figure 3.6a. In the case of the operation curves obtained with all $\eta_i = 1$, the maximum COP is found under off-design operation of the ejector only for $T_{amb} = 15$ [°C] (Fig. 3.6a). Interestingly, in Figures 3.6b and 3.6c, the maximum COP point is found when the ejector operates at critical conditions, which is in contradiction with the previous remark. Further analysis then indicates that the maximum COP can be found at critical ejector operation even when all efficiencies are not equal to unity. To this end, Figure 3.7a shows operation curves for $T_{amb} = 25$ [°C] generated by varying one independent efficiency at a time (by default, $\eta_i = 1$). Plain and dashed curves indicate on-design and off-design operation, respectively. As can be seen, the maximum COP is found at critical conditions not only in the case where $\eta_i = 1$ but also when the expansion processes are non-ideal in the primary nozzle. Actually, the optimal COP being located at critical

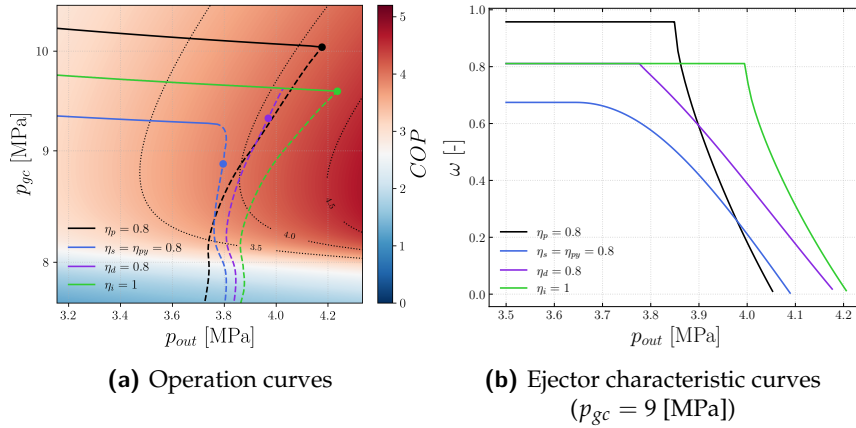


Fig. 3.7 Operation curves and characteristic curves for $T_{amb} = 25$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]) with different sets of efficiencies. Unless indicated otherwise in the legend, all efficiencies are set to unity. In Fig. 3.7a, the plain and dashed curves indicate on-design and off-design regime, respectively, and the dotted lines are iso-COPs.

3 | Performance analysis of the ERS

operation is mostly due to the fact that the off-design part of the ejector characteristic curves becomes very steep as the efficiencies get close to unity. This can be seen in Figure 3.7b, where the characteristic curves are plotted for different configurations of the efficiencies for $p_{gc} = 9$ [MPa]. The η_p efficiency does not modify the sharpness of the transition between on- and off-design regimes, unlike η_s , η_{py} and η_d , which is why the optimal COP for $\eta_p = 0.8$ in Figure 3.7a is found at the critical conditions as in the case where $\eta_i = 1$. The steepness of the characteristic curves translates into a sharp transition between the two regimes in the operation map, as there is a strong decrease in ejector performance as soon as the device goes under off-design. The η_s , η_{py} and η_d efficiencies reduce the sharpness of this transition (Fig. 3.7b) and thereby displace the optimal COP point to the off-design regime of the ejector. From Figure 3.6, the highest COP in the maps are found towards the right, at the limit of the non-physical region. Therefore, the best ejector would be one whose operation curve can go as far right of the map as possible (p_{gc} has to be relatively low as well). As per Figure 3.7a, the optimal strategy is then to reduce the entropy generation (have the η_i as high as possible) within the device, as any decrease in one of the efficiencies shifts the operation curve to the left. As a side note, even if all efficiencies are set to unity, entropy is still generated in the modeled mixing process because of the shock waves, which is why the operation curves in Figure 3.6 do not reach the limit of the non-physical region (in dark gray). Additionally, it is important to keep in mind that a real ejector always has $\eta_i < 1$, therefore it should be expected that the optimal COP will in practice always be found under off-design operation of the ejector.

3.4.3 Influence of the geometry on the COP

As a second step to determine the potentially best operation of the ERS, it is proposed to focus on the impact of the ejector geometry on the ERS performance. To this end, several maps of the COP as a function of the gas cooler pressure and the TAR A_y/A_t are generated. Note that the value of p_{gc} determines a single value of p_{out} along the operation curve (Fig. 3.6), so that the representation of the COP maps in the space ($p_{gc} - A_y/A_t$) is unambiguous. It is chosen to focus on the ratio of secondary to primary throat area since it constitutes the main design parameter of the ejector. The primary nozzle exit is first kept equal to the primary throat as in [109, 155]. Note that all maps presented in this section are done with the real ejector model calibrated on the experiment of Zhu et al. [155]. Figure 3.8 shows the

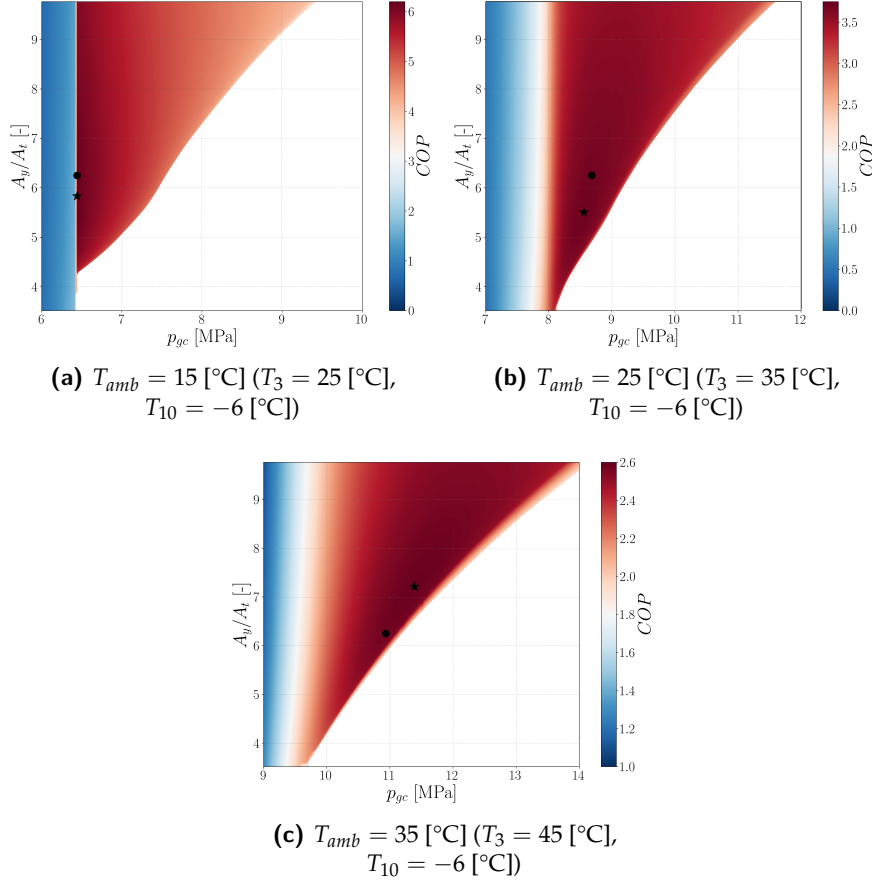


Fig. 3.8 Maps of the COP as a function of the gas cooler pressure and the TAR. The dot and star indicate the locations of the maximum COP with the original geometry of [155], and the global maximum COP, respectively.

generated maps for the three studied ambient temperatures. The maximum COP with the original geometry of [155] ($TAR = 6.25$) and the global maximum COP are indicated on the different maps; the global maximum COP being the maximum COP obtained by optimizing the original geometry according to the TAR. The optimal geometry appears to depend on the ambient temperature in a non negligible manner, also implying significantly different operation pressures with respect to the base geometry. Under sub-critical operation (Fig. 3.8a), the maximum COP is found at the saturation

3 | Performance analysis of the ERS

Maximum COP	T_{amb} [°C]	15	25	35
Geom. of [155] (TAR=6.25)		6.17	3.68	2.57
O.G. for $T_{amb} = 15$ [°C] (TAR=5.83)		6.18	3.69	2.55
O.G. for $T_{amb} = 25$ [°C] (TAR=5.50)		6.17	3.70	2.53
O.G. for $T_{amb} = 35$ [°C] (TAR=7.21)		6.12	3.64	2.59

Table 3.2 Maximum COP obtainable along the operation curve for the three studied T_{amb} values and for the base (Zhu et al. [155]) and optimal geometries (O.G.) obtained for those temperatures (Fig. 3.8). Efficiencies are calibrated on [155].

discontinuity (i.e., at $p_{gc} = 6.43$ [MPa], as discussed in Section 3.4.2), which is consistent with Figure 3.6a. In that case, it is then best for point 3 (Fig. 3.2) to be at saturated liquid conditions (raising or lowering p_{gc} from $p_{gc} = 6.43$ [MPa] –at constant T_3 – deteriorates the COP).

Table 3.2 summarizes the maximum COP values indicated in Figure 3.8. To estimate the sensitivity to the geometry, the maximum obtainable COP for each of the three optimal geometries (depending on T_{amb}) for each value of T_{amb} is also shown in Table 3.2. As can be seen, although there is a non negligible difference in optimal TAR depending on the ambient temperature, it appears that the performance gain compared to the base case, or even with respect to the optimal geometry for a different T_{amb} , is marginal. For example, if one were to operate the cycle at $T_{amb} = 35$ [°C] with the ejector that has the optimal TAR for $T_{amb} = 25$ [°C], one would only get a decrease in COP of about 2.4% compared to using the optimal TAR for $T_{amb} = 35$ [°C]. Note however that the TAR should nonetheless lie within a certain acceptable range, as the performance of the ejector may quickly deteriorate [150]. Notice that since the optimal TAR does not vary monotonously with T_{amb} (Fig. 3.8), the maximum COP does not vary monotonously either with the optimal geometries at fixed T_{amb} in Table 3.2.

Although the TAR seems to have little impact, it is possible that the ejector size may play an important role. It is then proposed to determine the ejector dimensions for a fixed cooling power $\dot{Q}_{ev} = 30$ [kW], but operating at different ambient temperatures. Table 3.3 summarizes the primary and secondary throat diameters (respectively, D_t and D_y) of the ejector operating at the maximum COP point with the optimized geometry for each T_{amb} (the operating points highlighted by the stars in Fig. 3.8). As can be seen, the change in dimensions is small from case to case, as there is a difference of

	$T_{amb} = 15 [^{\circ}\text{C}]$	$T_{amb} = 25 [^{\circ}\text{C}]$	$T_{amb} = 35 [^{\circ}\text{C}]$
$p_{gc} [\text{MPa}]$	6.44	8.56	11.4
$\dot{m}_p [\text{kg/s}]$	0.191	0.245	0.280
$\dot{m}_s [\text{kg/s}]$	0.126	0.131	0.136
$\omega [-]$	0.660	0.534	0.483
$D_t [\text{mm}]$	2.74	2.76	2.39
$D_y [\text{mm}]$	6.62	6.47	6.42

Table 3.3 Gas cooler pressures, ejector mass flow rates and throat diameters for optimal operation (Fig. 3.8) at each ambient temperature. The ejector model is calibrated on Zhu et al. [155].

less than 0.4 [mm] in primary throat diameter between the extreme cases $T_{amb} = 25 [^{\circ}\text{C}]$ and $T_{amb} = 35 [^{\circ}\text{C}]$. Such small dimension differences may not justify the implementation of multiple ejector geometries within the ERS and a single geometry that performs relatively well for the range of ambient temperatures of the application could be considered. However, in most refrigeration applications, the required cooling power is not constant, but is rather often directly dependent on the ambient. Then, significant changes in the ejector size are to be expected. For example, if one would operate at $T_{amb} = 25 [^{\circ}\text{C}]$ and the cooling power is reduced from $\dot{Q}_{ev} = 30$ [kW] to $\dot{Q}_{ev} = 15$ [kW], the primary throat diameter should, to remain on the maximum COP operation point, be reduced from $D_t = 2.76$ [mm] to $D_t = 1.96$ [mm]. For this reason, multi-ejector modules and needle regulated ejectors constitute compelling control technologies. While the first one may contain a discrete number of ejector geometries tailored for specific operating conditions, the latter can precisely regulate the primary mass flow rate, but the TAR is then imposed. So far, only a converging primary nozzle has been considered. At constant secondary throat area A_y (base geometry), Figure 3.9a then shows the COP map for $T_{amb} = 25 [^{\circ}\text{C}]$ as a function of the gas cooler pressure and the primary exit to throat area ratio A_e / A_t , with the efficiencies calibrated on [155]. The white region corresponds to invalid (non physical) predictions of the ejector model. As can be seen, the COP appears to be strongly dependent on A_e / A_t , but this result is actually biased because as A_e gets bigger, the expansion of the primary stream after the throat takes place within the primary nozzle, and $\eta_p > \eta_{py}$ as per the calibration on [155]. Figure 3.9b displays a similar COP map but with the η_{py} efficiency now set equal to $\eta_p = 0.95$. As can be

3 | Performance analysis of the ERS

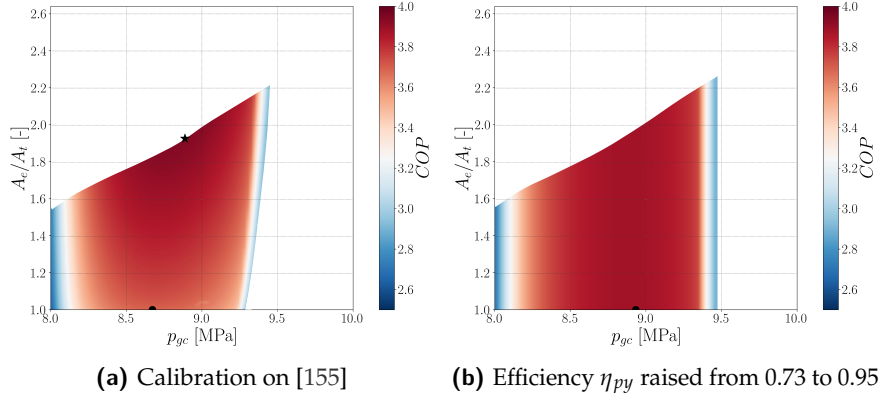


Fig. 3.9 Maps of the COP as a function of the gas cooler pressure and A_e/A_t for $T_{amb} = 25$ [°C], $T_{cool} = 4$ [°C] ($T_3 = 35$ [°C], $T_{10} = -6$ [°C]). The dot and star (Fig. 3.9a) indicate the locations of the maximum COP with the original geometry of [155], and the global maximum COP, respectively.

seen, if one has $\eta_p = \eta_{py}$, the COP becomes strictly independent of A_e/A_t . Nonetheless, the result of Figure 3.9a still contains some physical insight, since expanding the primary within a diverging part may reduce the entropy generation of this expanding process compared to further expanding it in the mixing chamber, and should lead to an overall higher COP. Actually, it is found that the maximum COP point in Figure 3.9a (indicated by the star) is located at the limit of the non-physical region, the latter corresponding to a re-compression of the primary stream directly after exiting the primary nozzle, which is not handled by the thermodynamic model. This case (the star) therefore corresponds to having a primary nozzle that can expand the primary stream to the mixing pressure exactly. However, a thorough analysis should be done with CFD tools and therefore exceeds the scope of the present work.

3.4.4 Analysis of the ejector regime

In this section, it is proposed to analyze the operating regime of the ejector for the base geometry and each of the optimal geometries for the three ambient temperatures of interest (i.e., the same cases as shown in Table 3.2). To this end, Figure 3.10 shows the characteristic curves (ω vs p_{out}) for each case, where the operation points are highlighted with a diamond marker. It can be noticed that all operation points are relatively close to

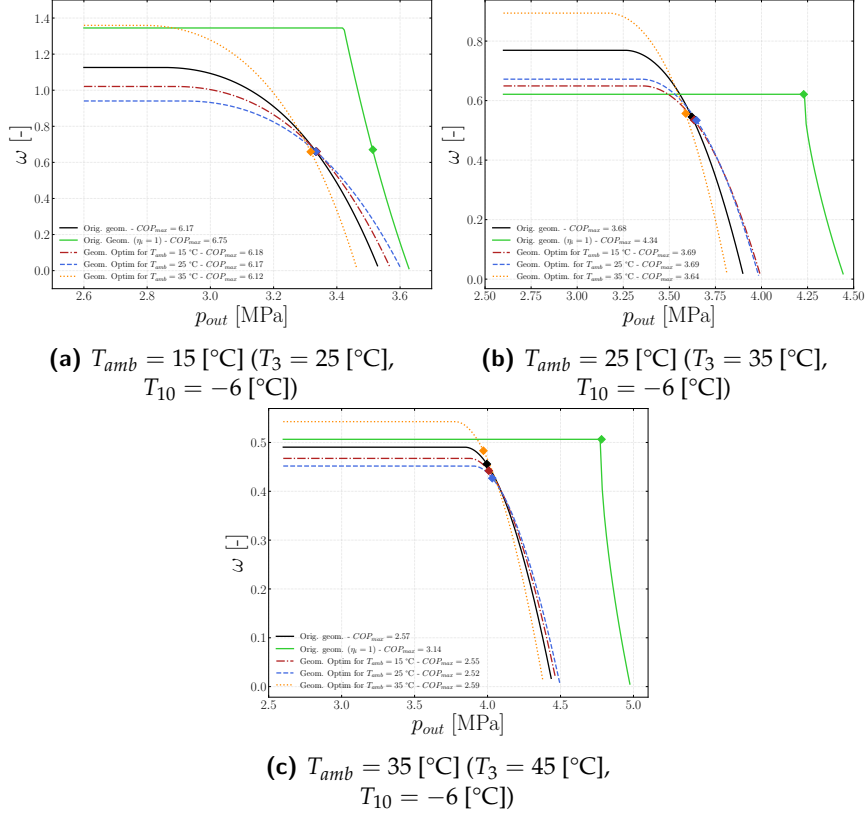


Fig. 3.10 Maximum COP operation points (diamonds) on their characteristic curve for each optimal geometry and for various ambient temperatures. The case with all $\eta_i = 1$ is also shown for reference. The operation points correspond to those in Table 3.2.

each other for each T_{amb} . In addition, disregarding the case with $\eta_i = 1$, the operation points with higher compression ratios (higher p_{out}) do not necessarily have higher COPs (Fig. 3.10b and 3.10c). Likewise, there is no apparent correlation between how close an operation point is to the critical operation point of the ejector (on-/off-design limit) and the COP. For example in Figure 3.10c, the case with the geometry optimized for $T_{amb} = 35$ [°C] appears to be "more off-design" than the other cases, but actually performs better. The general observation is then that all cases seem to have relatively similar entrainment ratios. One can see in Figure 3.10a that the case with $\eta_i = 1$ is under far off-design regime, which is a

3 | Performance analysis of the ERS

requirement to match the entrainment ratio required by the cycle (Fig. 3.5). Matching between cycle requirement and ejector performance is the most important factor when designing an ERS, and this requires a non-trivial analysis such as the present one. From this analysis, it is also clear that there is no incentive to operate the ejector under on-design regime for applications where the ejector is used as an expansion device in a refrigeration cycle.

3.4.5 High temperature gas cooler

So far, the present study indicated that the maximum COP is found when the ejector operates under off-design (or possibly critical) regime. However, it was reported in the work of Metsue *et al.* [109] that the optimal operation is found under on-design operation of the ejector, which is in contradiction with the present argument. Actually, despite the cycle configuration being slightly different, the main difference is that the cycle presented in [109] is operating as a heat pump to generate heat, not for refrigeration purpose. The hot source temperature is then higher. It is therefore proposed to analyze the operation of the present ERS with a hot source temperature of $T_{hot} = 65$ [°C] (as reported in [109]). Using the same temperature pinch at

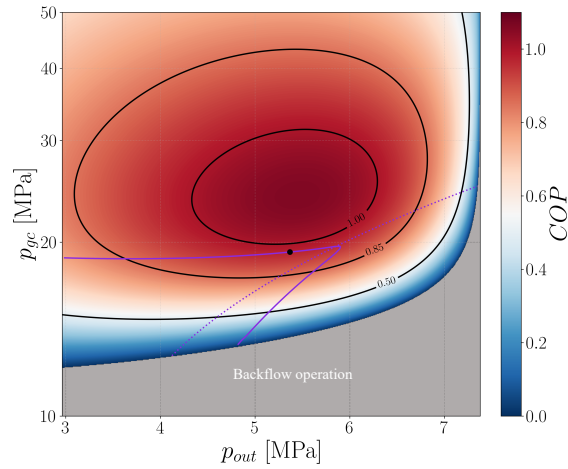


Fig. 3.11 Map of the COP as a function of the gas cooler pressure p_{gc} and the ejector outlet pressure p_{out} for $T_{amb} = 65$ [°C], $T_{cool} = 4$ [°C] ($T_3 = 75$ [°C], $T_{10} = -6$ [°C]). The purple line is the operation curve with the fitting for the ejector of [155]. The on-/off-design limit is plotted in dotted line and the maximum COP is highlighted with the dot.

the gas cooler as previously, one then gets that $T_3 = 75$ [°C] (Fig. 3.1). Figure 3.11 shows the generated COP map with the operation curve obtained using the ejector geometry of [155] ($TAR = 6.25$). As in Figure 3.6, the dotted line represents the limit between on- and off-design operation of the ejector. As can be seen, the maximum COP point along the operation curve (marked by the black dot) is found within the on-design region, which is in agreement with the conclusions of [109]. Therefore, based on the present observation along with the previous ones, one can deduce that as T_{hot} gets higher, the maximum COP point gets closer to on-design operation of the ejector (also consistent with Figure 3.10) until being found at critical operating conditions at a given temperature. Above said temperature, the maximum COP is found when the ejector operates under on-design regime. In the present configuration of the cycle ($T_{cool} = 4$ [°C] and ejector model calibrated on [155]), it is found that the switch from on- to off-design regime occurs at $T_{hot} \approx 60$ [°C] ($T_3 \approx 70$ [°C]).

3.5 Conclusions

In this work, an in-depth theoretical analysis of the operation of the classical ERS was performed using a thermodynamic modeling approach. A state-of-the-art ejector model was integrated within the cycle to generate COP maps and determine both what could be the optimal operation strategy for the cycle, and what would be the main design objectives for the ejector device. First, it was found that there exists an operation curve, which is the locus of the set of operating conditions that can allow steady state operation of the ERS. This means that, all other parameters being fixed by the application, the cycle cannot operate at any given set of gas cooler and ejector outlet pressures. The allowable sets of pressures are determined by the cycle requirements and the ejector internal physics. Then, the analysis showed that for an ejector with a realistic amount of entropy generation associated to the irreversible mixing phenomena, the maximum COP operation point is likely to be found when the ejector works under off-design regime. As the ambient temperature gets higher, the optimal operation point gets closer to the on-design operation of the ejector and can eventually shift to a full on-design operation if the temperature of heat rejection is higher than a certain threshold.

Secondly, it was found that the main design strategy for the ejector within the ERS is to minimize the entropy generation within the device. Indeed, it was observed that any decrease in any of the efficiencies of the thermody-

dynamic model should lead to a decrease in the maximum achievable COP of the ERS. In addition, it was found that, as entropy generation is reduced within the ejector, the maximum COP point gets closer to critical ejector operation. When the entropy generation becomes sufficiently small, the optimal operation point is found at critical operating conditions of the ejector. However, it was found that there is no benefit to operate the ejector under on-design regime (at pressures lower than that of critical operation regime) for refrigeration applications. In addition, optimizing the throat area ratio of the ejector yielded only little improvement of the COP. It is important to note that constant efficiencies were used to calibrate the ejector model, while it is expected those efficiencies should possibly be functions of the geometry and operating conditions. However, the authors believe that finding such correlations for the efficiencies constitutes a whole subject of research beyond the scope of the present work, certainly requiring the support of machine learning techniques (as in, e.g., [145]).

From this analysis, it is the authors' understanding that ejector design for refrigeration application should be done by accounting for the whole operation of the system, and not at the component level solely. Note also that the present work is focused on cooling applications, but as established in this paper, above a given hot source temperature threshold, the maximum COP is found when the ejector is under on-design regime, as reported in [109]. Therefore, a deep analysis of the cycle operating in heat pump mode could be done in the future. Additionally, future work could be done with CFD and machine learning tools to determine the influence of the different 2D/3D geometrical parameters of the ejector, such as, e.g., the primary nozzle divergent angle. This could allow to also support the development of correlations for the fitting efficiencies of the ejector model, or even directly optimize the geometry to minimize the entropy generation within the device.

4

Analysis of the Exergy Transfers in Subcritical and Transcritical CO₂ Ejectors and their Connection with the Performance of the Refrigeration Cycle

4.1 Foreword

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Abstract:

Ejector refrigeration systems (ERSs) operating with carbon dioxide are notoriously challenging from both design and operation perspectives. In particular, the ejector itself gives rise to special attention since it directly affects the performance of the global system. In this study, the connections between local exergy transfers within the ejector and global cycle performance are investigated by using a novel multi-scale numerical approach. Computational Fluid Dynamics (CFD) is used to generate accurate predictions of the ejector operation with access to the local flow and heat transfer features. The exergy tube analysis is applied onto the simulation results, linking local transfers within the ejector to the results at the component- and cycle-scale. A state-of-the-art ejector thermodynamic model is then calibrated onto the CFD results, and employed to determine the physically possible operation of the ERS. In addition, the metastability impact on the exergy transfers and overall system performance is investigated by comparing the CFD results of the classical Homogeneous Equilibrium Model with those obtained with the Homogeneous Relaxation Model. Notably, it is found that at fixed ejector inlet conditions, there exists an outlet pressure that maximizes the exergy transfers from primary to secondary streams. Interestingly, this work shows for the first time that the maximum exergy gain of the secondary stream appears to correlate with the maximum coefficient of performance of the system, independently of the on- or off-design operation of the ejector. Moreover, metastability generally deteriorates the performance at both scales. The results of the present study serve to pave the way towards better ejector design objectives.

4.2 Introduction

Research on carbon dioxide (CO₂) refrigeration systems has gained substantial attention in the recent years, mostly due to the shift towards natural refrigerants that is motivated by international agreements such as the 2016

Kigali amendment to the Montreal protocol, in which 159 countries committed to reduce the production and consumption of HFCs by more than 80% by 2045 [144]. The general safety of CO₂ (non-flammability and non-toxicity) and its low global warming potential and zero ozone depletion potential, come however at the expense of an overall lower performance of the refrigeration system compared to more traditional refrigerants [52]. The relatively low critical temperature of CO₂ (at 31 °C], close to the ambient) often leads, indeed, to the necessity to reach high (supercritical) pressures on the heat rejection side of the cycle. Consequently, such cycles are said to operate under *transcritical* regime, which leads to high expansion losses in the expansion valve [79].

Ejectors are favorable devices used to suck and compress fluids, which enable the use of CO₂ by recovering part of the exergy losses during the expansion. Figure 4.1 depicts the conventional ejector refrigeration cycle, which has been proven to achieve the most favorable coefficient of performance (COP) compared to other suggested configurations for CO₂ systems [142]. By discharging a high pressure primary fluid (coming from the gas cooler) into a primary nozzle, the low pressure fluid at the secondary inlet (coming from the evaporator) is entrained and compressed within the secondary nozzle. The outlet refrigerant exits the device with intermediate thermodynamic conditions, as a pre-compressed state, so that the compressor is able to work at a lower charge to provide the same cooling power.

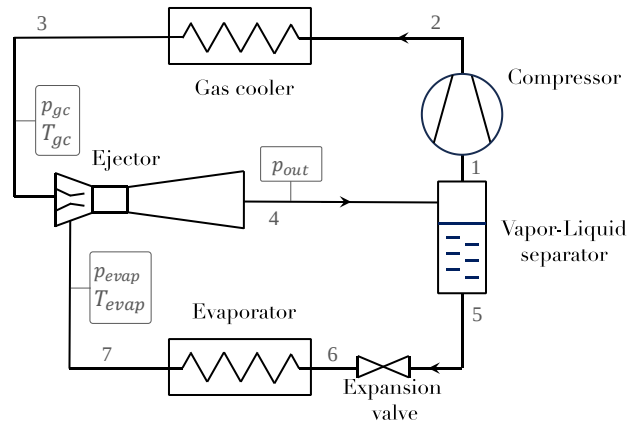


Fig. 4.1 Classical ejector refrigeration system. The different points are numbered for reference in the text.

Several studies compared the conventional transcritical CO₂ refrigeration cycle to its ejector-based counterpart [51, 87, 94, 102]. The studies all pointed out that the addition of the ejector in the cycle is favorable and exhibited potential to increase its COP. Notably, Elbel and Hrnjak [51] found out that the cooling capacity and the COP could be improved by up to 8% and 7%, respectively. Similarly, Li and Groll [87] studied the influence of operating parameters on the performance of the cycle and found that the COP of the transcritical CO₂ system could be improved by more than 16% by the addition of the ejector, for typical air conditioning operation conditions. Ejectors are nonetheless characterized by complex fluid dynamics and exergy transfer phenomena. Even though there has been significant advancements to understand the local flow behaviors of the device [34, 83, 84], a better understanding of the exergy exchanges/dissipation within the device and their relation with the global cycle performance are still required to design and operate ERSs properly (to obtain higher ejector efficiency and consequently enhanced system performance).

Several strategies can be adopted to study the performance and flow physics of the ejector specifically. The simplest approach is to use a thermodynamic (or 0D) model. Initially limited to single-phase modeling (e.g., [29, 85, 135]), advanced models able to predict real gas ejector operation under on- and off-design, were developed [6, 110, 143]. Recently, Metsue *et al.* [110] introduced the real choking phenomenology of the *compound-choking* into their thermodynamic model and demonstrated its fitting capability onto experimental data. Wang *et al.* [146] later proposed an alternative analytical model relying on only five parameters. Taking into consideration the position of the double-choking section, the authors defined three limit states to compute the critical entrainment ratio. Despite remaining limited to ideal gas ejectors, it was stated by the authors [146] that their model performed better than current ones available in the literature. It should however be noted that in [146], fitted characteristic curves reported in [110] were compared to the results of an experimental run different from the one used in said reference, thus showcasing a lesser performance of the compound-choking model compared to its actual capabilities. To obtain more detailed information about the internal flow physics, Computational Fluid Dynamics (CFD) can be used. Several works have then been done to characterize the flow topology with respect to the operating conditions (e.g., [61, 84]), or to study the mixing chamber geometry, shock wave formation and irreversibilities [48, 83, 147, 148]. In particular, Lamberts *et al.* [83] extended the transport tube analysis of Meyers and Meneveau [114] to

exergy transport tubes, in the context of air ejectors. This analysis allowed to determine the locations and amplitudes of the local exergy transfers and losses within the ejector. Metsue *et al.* [112] later performed a similar exergy analysis for the first time on a CO₂ ejector, using this time the SU2 [119] solver, and found that the exergy losses within the secondary stream quickly overpower the exergy gain provided by the primary stream as the ejector goes into the on-design regime.

In the particular case of two-phase CO₂ ejectors, additional care has to be taken with regards to the flashing phenomenon, as the latter is known to occur under thermodynamic non-equilibrium and thus introduce a metastable phase (liquid) along the flow expansion depending on the inlet conditions; this can severely affect both the flow topology and the flow rates [113] as the speed of sound in a two-phase flow is strongly dependent on the mixture composition. Indeed, as both liquid and vapor phases are present, additional assumptions and modeling are required to solve the system of partial differential equations (PDEs). The Homogeneous Equilibrium Model (HEM) constitutes the simplest approach, and defines the vapor/liquid mixtures as a pseudo-state that is both in mechanical and thermodynamic equilibrium. However, the HEM can suffer from large discrepancies with the experiment as the primary inlet temperature becomes subcritical [122]. Those discrepancies are mostly attributed to the thermodynamic equilibrium hypothesis rather than to the mechanical one [40]. More advanced two-phase models have been implemented [21, 70, 89, 95, 113] to tackle this issue. Among the proposed non-equilibrium models, the Homogeneous Relaxation Model (HRM) [18] is a 4-equation model that offers a compelling approach as it only assumes mechanical equilibrium of the phases [129]. The HRM has been used to simulate CO₂ ejectors both in 1D [8, 98] and 2D/3D using CFD tools [70, 121], and was for the first time adapted in a density-based CFD solver (more adequate for highly compressible flows [56]) by Metsue *et al.* [113]. Note at this stage that the majority of experimental two-phase CO₂ ejector measurements documented in the open literature typically only includes mass flow rates, inlet/outlet pressures and temperatures, sometimes with limited wall pressure measurements (e.g., [69, 63]) or visualizations of moderate quality [90, 156]. Most studies focused indeed on the effect of the ejector on the cycle rather than on the fine characterization of the ejector. This consequently makes the validation of ejector numerical models difficult and globally impedes on progress. Having access to local flow quantities (e.g., detailed pressure profile or local velocity field) could give precious insight onto the nature of the physical phenomena taking place depending

on the operation of the device, leading to better numerical modeling.

Many studies have been conducted in order to assess the performance of the Ejector Refrigeration System (ERS) at the cycle/system scale. Fangtian and Yitai [58] conducted an exergy analysis, which identified critical parameters such as entrainment ratio, gas cooler outlet temperature, and heat rejection pressure, that optimize the cycle operation. Using the Dymola software, Metsue et al. [109] analyzed the impact of the ejector geometry on the performance of a transcritical CO₂ ejector cycle, and found that the maximum COP is reached when the ejector operates under on-design regime. Some works also involve, at some level, the internal flow physics of the ejector with the performance of the system. Besagni et al. [16] combined CFD results of a single ejector with a 0D model of an ejector refrigeration cycle and studied the choice of refrigerant on the COP of the system for five ejector geometries. The authors [16] used this approach to link the local flow features and ejector geometry to the system performance. Later, Metsue et al. [111] employed their ejector thermodynamic model [110] to predict the performance of a CO₂ ERS. The maximum COP was not reached when the ejector operates at critical conditions, but mostly when the device is under off-design regime at typical gas cooler outlet temperatures (between 25 and 45 [°C], and moving towards on-design regime (as in [109]) as said temperature is raised).

As deduced by the present literature survey, many studies have decided to either study the ERS at the system scale, or at the component level. However, few attempts have been done to bridge the gap between the two approaches and to the best of the authors' knowledge, the global performance of the ERS has never been associated to the local exergy transfers within a flashing CO₂ ejector. In the present work, it is then proposed to use a multi-scale approach by combining for the first time wall-resolved Favre-Averaged Navier-Stokes (FANS) simulations and thermodynamic modeling to investigate the relationship between local- and global-scale behaviors. The exergy tube analysis developed by Lamberts et al. [83] is first applied to the numerical results of the transcritical CO₂ ejector considered experimentally by Bodys et al. [20]. After calibration onto the CFD results, the thermodynamic model of [111] is used to predict the operation of a typical ERS for various operating pressures and temperatures. The link between local (component or ejector scale) and global (cycle or system scale) performance is then investigated by combining the ejector exergy analysis of the CFD results with the COP predictions of the cycle obtained with the thermodynamic model. Then, a similar analysis is brought to subcritical

operations, using this time the HRM, which enables to shed light onto the influence of metastability onto the ejector operating regime, local exergy transfers and, for the first time, on the global performance of the ERS. This work serves to provide a better understanding of how the cycle benefits from the ejector at a physical level, which can pave the way towards better ejector design objectives and operation strategies.

4.3 Numerical methodology

In this section, the general analysis procedure is first described in Section 4.3.1. The geometry, operating conditions and meshing are presented in Section 4.3.2, followed by the description of the CFD methods, exergy analysis tools and cycle/ejector thermodynamic modeling in Sections 4.3.3, 4.3.4 and 4.3.5, respectively.

4.3.1 General procedure

As stated previously, the current approach is based on the comparison between CFD results on the one hand, and thermodynamic modeling on the other. Figure 4.2 shows a schematic view of the strategy employed in this work. Note at this stage that this work constitutes a theoretical analysis. Given a number of ejector inlet and outlet conditions (pressure and temperature at the inlets and pressure at the outlet (Fig. 4.1)), CFD is performed to generate ejector characteristic curves (as described in, e.g., [110]). With those results as a basis, the analysis is then continued at local and global scales. On the local –ejector– scale, the exergy tube analysis [83] is applied to determine the conditions that lead to the optimal exergy transfers. On the global –ERS– scale, the ejector thermodynamic model [110] is calibrated onto the CFD characteristic curves to ensure that the cycle operates with an ejector with the same integral behavior than the one

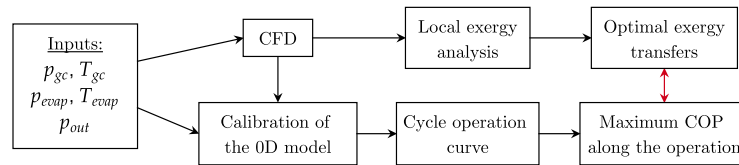


Fig. 4.2 Flowchart of the procedure that is applied in the present work to determine if there is a correlation between optimal exergy transfers within the ejector and maximum COP of the cycle (red arrow).

used to conduct local exergy transfers analysis. The operation curve in the $(p_{gc} - p_{out})$ domain is then obtained by using the ejector thermodynamic model (Section 4.3.5) to find the set of gas cooler and ejector outlet operating pressures that are achievable by the device, as thoroughly explained in [111]. It is then possible to find the conditions that lead to a maximum COP along the operation curve, and compare them with the conditions that lead to the optimum exergy transfers.

4.3.2 Geometrical modeling and operating conditions

A single ejector geometry provided by [20] is used and corresponds to the experimental setup of Haida *et al.* [68]. In the present work, experimental mass flow rate measurements are used for validation purposes only, as the core of the analysis remains numerical. The main dimensions of the axisymmetric device are given in Table 4.1. For the thermodynamic model which incorporates the 0D ejector model, only the primary nozzle throat, the exit area, and the cross-section area of the constant area duct are needed. With regards to the operating conditions for CFD simulations, both subcritical and supercritical primary inlet conditions are considered, which are summarized in Table 4.2. Two supercritical temperatures are tested for four primary inlet pressures. Although the two temperatures are close to each other (i.e., 35 and 36 [°C]), notable differences will be visible in the following, as the operation of the ERS is quite sensitive to T_{gc} . For each set, several outlet pressures are evaluated, to cover both the on- and off-design regimes. This enables subsequent proper calibration of the thermodynamic model. In addition, one subcritical temperature (for 4 primary pressures) is studied, which will also be used to determine the influence of metastability on the device and system performance. Metastability effects are mostly expected for low nozzle inlet temperatures [122] (also implying a low gas

Parameter [Unit]	Dimension
Primary nozzle inlet diameter [mm]	3.80
Primary nozzle throat diameter [mm]	1.41
Primary nozzle exit diameter [mm]	1.58
Constant area duct diameter [mm]	3.25
Constant area duct length [mm]	16.25
Diffuser angle [°]	5.00
Diffuser outlet diameter [mm]	8.40

Table 4.1 Dimensions of the ejector.

T_{gc} [°C]	p_{gc} [MPa]				p_{out} [MPa]			
25	6.45	6.55	6.7	6.95	2.50	2.60	...	3.40
35	8.25	8.50	8.75	9.00	2.80	2.90	...	3.80
36	8.50	8.75	9.00	9.25	2.80	2.90	...	3.80

Table 4.2 Operating conditions used for the CFD simulations. The ellipses (...) indicate intermediate values, equally spaced by 0.1 [MPa].

cooler pressure within the CO₂ ERS), hence the choice of $T_{gc} = 25$ [°C]. The secondary inlet is set at constant pressure and temperature ($p_{evap} = 2.8$ [MPa], $T_{evap} = 7.5$ [°C]) since the interest is focused on the determination of the optimal operating pressures at the compressor inlet/outlet. The secondary conditions are then assumed to be fixed by the application, here for a typical air-conditioning purpose.

4.3.3 CFD modeling and validation

The FANS simulations are conducted using SU2 (version 7.3.1), which is a real-gas density-based CFD solver. In SU2, the PDEs are discretized via a finite volume approach. As reported in [119], this method employs a standard edge-based structure on a dual grid, where control volumes are constructed using a median-dual, vertex-based approach. The interested reader is invited to refer to the original article of Palacios *et al.* [119] for detailed information about the FANS equations and their specific implementation within SU2.

Since flashing CO₂ ejectors involve the presence of a vapor/liquid mixture, additional assumptions are required in order to solve the system of PDEs. In what follows, both the HEM and HRM are employed. In HEM, mechanical and thermodynamic equilibria are assumed, which leads to the well-known definition of the vapor quality x . In HRM, only mechanical equilibrium is assumed, as the –metastable– liquid is vaporized with a delay to reach equilibrium, which is treated as a relaxation process.

In practice, an additional PDE has to be solved for the transport of the vapor phase:

$$\frac{\partial}{\partial t} (\rho x) + \frac{\partial}{\partial z_j} (\rho u_j x) = -\rho \frac{x - x_{eq}}{\theta}, \quad (4.1)$$

with ρ the density, u_j the velocity components and θ the relaxation time. The j and eq subscripts indicate spacial coordinate and equilibrium quantity, respectively. Specific correlations have been developed for the relaxation

time [70, 98], but as argued in Metsue *et al.* [113], such correlations are mostly case-specific with regards to both geometry and operating conditions. Therefore, only constant relaxation times are used in the present theoretical study, where the density-based algorithm of [113] is employed along with their tabulated Equation of State (EoS). The latter EoS is based on a quad-tree algorithm that combines piece-wise bicubic interpolation with local refinement in the state space. Each HRM simulation is initialized with the HEM solution and integrated in time until convergence. Note however that the HRM is activated within the primary nozzle only. This is done in order to accelerate the convergence of the solution, and based on the assumption that metastability is mostly present within that part, near the vicinity of the throat where the flashing process begins and the quality gradient is high. The Menter Shear Stress Transport model [107] ($k - \omega$ SST) is used for the turbulence closure, which is motivated by its performance in aligning with experimental data, exhibiting good agreement for both local and global flow characteristics for perfect and real gas ejector flows [36, 84]. The second-order classical Roe scheme [130] is employed to integrate the convective fluxes, and the gradients for computing the viscous fluxes are derived using the Green-Gauss method. For HEM simulations, an Euler implicit time integration scheme (first-order) is utilized, with local time-stepping for faster convergence. For HRM simulations, the pseudo-time integration relies on an Euler explicit scheme (first-order) since, as explained in [111], the implementation of an implicit formulation is intricate as it would involve complex thermodynamic derivative terms. For Euler implicit simulations, a CLF number of 15 was used, whereas in Euler explicit simulations, the CFL was limited to 0.5 to ensure stability.

Total pressures and temperatures are prescribed at primary and secondary inlets of the ejector, whereas the static pressure is prescribed at the outlet. In addition, both inlet and outlet boundary conditions are characteristic-based (non-reflective), in order to inhibit the influence of spurious reflection waves on the solution convergence. Axisymmetric simulations are here performed. Hence a symmetry boundary condition is prescribed at the axis of the ejector. Note that in SU2, the axisymmetric solver assumes zero angular velocity, hence the PDEs are simplified and the third dimension, in the angular direction, does not have to be modeled to solve the system. For both HEM and HRM simulations, convergence is assumed when the relative difference in total mass flow rate between the inlets and the outlet of the ejector fell steadily below $5 \cdot 10^{-3}$.

For CFD simulations, a 2D mesh (Fig. 4.3) is generated with the GMSH

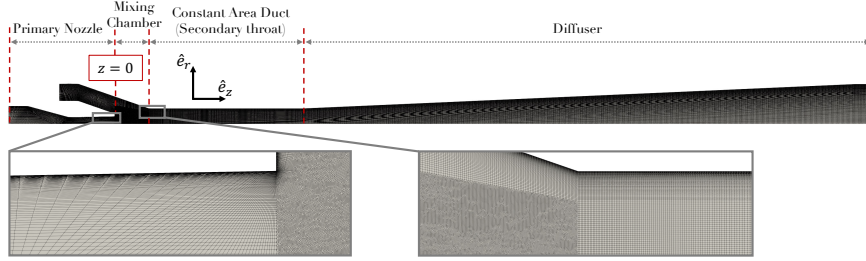


Fig. 4.3 Two-dimensional mesh of the ejector (axisymmetric view). By convention, the zero axial coordinate is set at the primary nozzle exit.

software. The mesh is composed of roughly 287 000 quadrilateral elements and is mostly structured, except within the mixing chamber in order to allow consistent relaxation of the cells dimensions near the primary nozzle tip. As shown in Figure 4.3, the mesh is refined towards the wall in order to have a maximum wall coordinate $y^+ \approx 1$, which is a requirement for low-Reynolds number turbulence closures. In addition, the mesh independence was verified by conducting a simulation with a mesh having twice as many elements in the $\hat{e}_z$ coordinate for the case ($T_{gc} = 35$ [°C], $p_{gc} = 8.50$ [MPa], $p_{out} = 3.40$ [MPa]). Note that the grid independence was verified in HEM and that it stays valid in HRM since all computation schemes are identical except for time integration, to which the independence of the solution was thus verified. Figure 4.4 displays the pressure profiles at the centerline using each mesh, where negligible difference is observed. A discrepancy

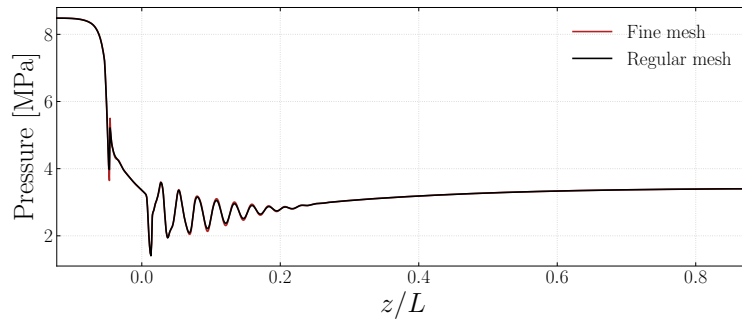


Fig. 4.4 Pressure profiles at the centerline of the ejector obtained with the regular and finer meshes ($T_{gc} = 35$ [°C], $p_{gc} = 8.50$ [MPa], $p_{out} = 3.40$ [MPa]).

of less than 0.2% was found for both primary and secondary mass flow rates between the two simulation results. Consequently, the original mesh (non-refined) was used to perform all subsequent simulations.

All computations are conducted on the clusters of the Digital Research Alliance of Canada. Each case is executed on two computation nodes, each equipped with 40 Intel Skylake cores running at 2.4 GHz. For HEM simulations, convergence was achieved after less than 12 hours wall time, whereas HRM simulations required around one week. This amounts to 960 and 13 440 CPU hours for HEM and HRM simulations, respectively.

In order to validate the solver for flashing CO₂ ejectors, primary and secondary mass flow rates ($\dot{m}_p$ and $\dot{m}_s$, respectively) obtained through HEM simulation are compared to the experimental data of a partial characteristic curve gathered by Bodys *et al.* [20]. The validation was not performed explicitly in HRM because it was found that for supercritical primary inlets, a very small relaxation time should be used. Otherwise, the flow would cross the spinodal limit (unstable limit [40]), and the physics of the HRM would not be valid anymore [113]. Thus, as in [70], for supercritical primary inlets, the HRM should behave like the HEM (almost identical simulation results). Both primary and secondary conditions are set to ($p_{gc} \approx 8.61$ [MPa], $T_{gc} \approx 35.5$ [°C]) and ($p_{evap} \approx 2.80$ [MPa], $T_{evap} \approx 7.5$ [°C]), respectively, with slight variation from case to case. Results are shown in Table 4.3, where the error is defined as:

$$\text{Err} = \frac{\zeta_{exp} - \zeta_{HEM}}{\zeta_{exp}}, \quad (4.2)$$

with ζ the quantity of interest. It can be observed that the HEM consistently under-predicts the primary mass flow rate by about 8%. Actually, the HEM

p_{out} [MPa]	$\dot{m}_{p,HEM}$ [g/s]	$\dot{m}_{p,exp}$ [g/s]	$\text{Err}_{\dot{m}_p}$ [%]	$\dot{m}_{s,HEM}$ [g/s]	$\dot{m}_{s,exp}$ [g/s]	$\text{Err}_{\dot{m}_s}$ [%]	ω_{HEM} [-]	ω_{exp} [-]	Err_ω [%]
3.283	66.01	71.90	8.29	35.56	33.36	-6.59	0.539	0.464	-16.09
3.390	63.88	69.54	8.14	31.60	32.11	1.59	0.495	0.462	-7.10
3.477	64.08	69.98	8.43	27.70	29.76	6.92	0.432	0.425	-1.62
3.563	64.05	69.83	8.28	23.48	27.35	14.15	0.367	0.392	6.41
3.825	63.63	69.57	8.54	12.93	19.58	33.96	0.203	0.282	27.81

Table 4.3 Predictions of the primary and secondary mass flow rates and comparison with the experimental data of [20].

systematically under-predicts mass flow rates since it predicts the smallest speed of sound among two-phase models [42]. Metastability phenomena may then contribute to this deviation, as it tends to increase the mass flow rate within the nozzle [113]. Alternatively, this discrepancy could be the results of losses between the pressure and temperature probes and the primary inlet. On the other hand, the secondary mass flow rate $\dot{m}_s$ shows relatively good agreement with the experiments, with errors ranging from -6.5% to 34%, which is typical for transcritical CO₂ ejectors. Secondary mass flow rate discrepancies between the HEM and experimental measurements ranging between 5% and 35% were reported in [70], and between 20% and 45% in [63], for similar operating conditions. Consequently, the entrainment ratio ω exhibits a similar error range. It is also noteworthy that the present solver has been already carefully validated in [113] for CO₂ flashing nozzles.

4.3.4 Exergy tube method

The exergy tube analysis of Lamberts *et al.* [83] is used to study the exergy fluxes between primary and secondary streams, and then assess the exergy gain of the secondary stream. Thorough explanations regarding the derivation of the related equations can be found in the original reference [83], as only a summary is provided here. The exergy tube is constructed by a set of transport lines that are, at any point, tangential to the mean flow exergy flux F_{ξ} , which can be expressed as [83]:

$$F_{\xi,j} = \rho u_j \xi_t + (q_j + q_j^t) \left(1 - \frac{T_{\text{ref}}}{T} \right) - \tau_{ij} u_i - \tau_{ij}^t u_i, \quad (4.3)$$

where $\xi_t = (h_t - h_{\text{ref}}) - T_{\text{ref}}(s - s_{\text{ref}})$ is the total specific exergy (h is the enthalpy and s the entropy), q is the heat flux and τ is the viscous stress tensor. The t subscript indicates total quantities, whereas the t superscript indicates turbulent quantities. The reference state (indicated by the ref subscript) is selected to correspond to the secondary inlet state [83]. Note that unlike in the case of a classical stream tube (mass transport tube), there are losses, so that the total exergy entering the tube is higher than that exiting the tube, in virtue of the second principle. The exergy losses can then be expressed as:

$$\Phi = \tau_{ij} \frac{\partial u_i}{\partial z_j} + \tau_{ij}^t \frac{\partial u_i}{\partial z_j} - (q_j + q_j^t) \frac{\partial T}{\partial z_j}. \quad (4.4)$$

4 | Optimal ejector exergy efficiency and COP

From Equation (4.3), the dimensionless cumulative transfer of total exergy I_{ξ} can be expressed as:

$$I_{\xi}(z) = \frac{\iint_{S(z)} F_{\xi,j} n_j ds}{\dot{m}_p \xi_{t,gc}}, \quad (4.5)$$

where n_j is the unit normal to the dividing streamline pointing towards the secondary stream and $S(z)$ is the dividing surface from 0 to z (axial direction). Figure 4.5 illustrates the relevant notations. The dividing surface then corresponds to the surface separating the primary stream from the secondary stream, that is, the mass transport tube emanating from the surface between the nozzle tip and the ejector axis. In Equation (4.5), the exergy flow is normalized by the primary inlet exergy flow (i.e., $\dot{m}_p \xi_{t,gc}$). Consequently, if I_{ξ} reaches unity, it means that all of the exergy of the primary stream has been transferred to the secondary stream (hypothetical case).

Similarly, the dimensionless cumulative exergy destruction in the secondary stream Π can be expressed as:

$$\Pi(z) = \frac{T_{\text{ref}} \iiint_{V_2(z)} \Phi / T dV}{\dot{m}_p \xi_{t,gc}}, \quad (4.6)$$

with $V_2(z)$ the volume occupied by the secondary stream, between the dividing surface and the wall, between sections 0 and z . By combining the secondary exergy gains (I_{ξ}) and losses (Π), one may then express the

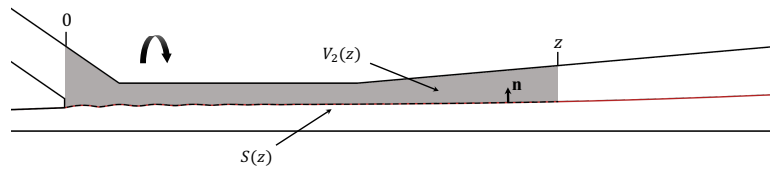


Fig. 4.5 Two-dimensional schematic displaying the relevant surfaces/volumes for the exergy tube analysis (axisymmetric view). The dividing streamline is plotted in red. The gray area is $V_2(z)$ and the dashed line $S(z)$.

dimensionless net exergy gain of the secondary stream Δ :

$$\Delta(z) = I_{\xi}(z) - \Pi(z) = \frac{\dot{m}_s \xi_{t,s}(z)}{\dot{m}_p \xi_{t,gc}}, \quad (4.7)$$

where the latter equality is derived naturally from the fact that the reference state is chosen to be that of the secondary inlet. In the present study, the dimensional net gain of exergy of the secondary stream $\delta(z) = \dot{m}_p \xi_{t,gc} \Delta(z)$ is also used to determine the actual exergy quantity that the secondary stream receives at a given operation point of the ERS.

4.3.5 Thermodynamic modeling

The classical CO₂ ERS (Fig. 4.1) is considered in this work in order to assess the expected performance of a refrigeration cycle. The modeling approach is similar to that of Metsue *et al.* [111] and constitutes a simple theoretical approach to the modeling of the system. Thus, only a brief description of the cycle and ejector models is recalled here. The assumptions with regards to the cycle are:

- The system operates at steady-state conditions. The mass conservation for the liquid phase at the separator level therefore imposes $x_7 = \dot{m}_p / (\dot{m}_p + \dot{m}_s) = 1 / (1 + \omega)$ (as per [111]).
- The temperature at the gas cooler exit T_{gc} is imposed by the ambient temperature (Tab. 4.2).
- The temperature at the evaporator outlet T_{evap} is imposed by the application (typical air-conditioning), and fixed to $T_{evap} = 7.5$ [°C]. The pressure at the evaporator is fixed to $p_{evap} = 2.8$ [MPa].
- No pressure losses occur across the gas cooler and the evaporator.
- Thermodynamic transformations inside the separator, expansion valve and ejector are adiabatic.
- The thermodynamic transformation within the compressor is assumed to be isentropic (pressures are prescribed at the compressor inlet and outlet by p_{out} and p_{gc} , respectively). In practice, the isentropic efficiency of a reciprocating compressor is typically in the range of 70%–90% [76], but well defined and simple parameters are chosen since the present analysis does not require more complexity.

4 | Optimal ejector exergy efficiency and COP

Based on those hypotheses, all states (points 1 through 7 in Figure 4.1) can be computed from two independent state variables using the EoS (obtained via COOLPROP [13]). Note that the pressures at the gas cooler and the ejector outlet (p_{gc} and p_{out} , respectively) are kept as parameters to conduct the forthcoming parametric analyses. Hence, those are inputs to be specified in order to solve the system of equations. In addition, the entrainment ratio and the COP are given by [111]:

$$\omega = \frac{h_1 - h_3}{h_7 - h_5}, \quad (4.8)$$

and

$$COP = \omega \frac{h_7 - h_5}{h_2 - h_1} = \frac{h_1 - h_3}{h_2 - h_1}. \quad (4.9)$$

Note that in this study, the cooling capacity does not need to be specified, by construction of the model. Only the *ratio* of evaporator mass flow rate to gas cooler mass flow rate (i.e., the entrainment ratio of the ejector) is required to determine the cycle performance. In order to obtain the operation curve of the ERS, one must then use the ejector thermodynamic model to predict the actual performance of the ejector. As described by Metsue et al. [111], the operation curve is defined by the set of operating conditions (here, the set of p_{gc} and p_{out}) that can allow steady-state operation of the cycle. In practice, this means that for such specific operating conditions, the ejector must provide an entrainment ratio that matches the requirements of the cycle. The thermodynamic model of Metsue et al. [110] is therefore used to predict the entrainment ratio of the ejector ω . This ejector model was thoroughly described and validated against experimental measurements in the previous works of Metsue et al. [110, 109]. The interested reader is invited to review these two references for further information. Its main assumptions and features are summarized below:

- The flow is 1D steady and adiabatic. Negligible velocities are assumed at both the inlets and the outlet.
- Isentropic efficiencies are employed to account for friction losses: η_p within the primary nozzle (wall friction), η_{py} for the primary stream within the mixing chamber (due to shearing with the secondary stream), η_s for the secondary stream within the mixing chamber, and η_d for the diffuser. Additionally, a loss coefficient η_m is utilized to address mixing losses between the primary and secondary streams.

Please refer to [110] for detailed information.

- The primary and secondary streams are assumed to remain distinct until they reach a specific section within the constant area duct, where their pressures are considered equal, and at which the mixing phenomenon begins.
- Mass and total enthalpy conservation equations are applied between each section, along with the equation of state provided by COOLPROP and isentropic efficiency relations. The momentum conservation equation is also utilized for handling the mixing process.
- The double choking of the ejector is modeled by the compound-choking theory [14].

4.4 Results and discussion for transcritical operations

In this section, the ERS is studied under transcritical operations, implying that the CO₂ at the exit of the gas cooler is at a supercritical state. In Section 4.4.1, the thermodynamic model is used to calculate the operation curve. Then, the exergy analysis at the local scale is conducted in Section 4.4.2, which enables to compare the performance at both ejector and system scales.

4.4.1 Operation curves

The first step of the present analysis consists in calibrating the 0D model onto CFD results. Note that in this section, only the HEM is employed. As per Table 4.2, two gas cooler outlet temperatures are studied, for four different gas cooler pressures. In addition, the four p_{gc} values allow to cover the range of operating conditions that can be expected in such an ERS. Figure 4.6 shows the results of the calibration process. It can be seen that a very good fitting is obtained. Table 4.4 gives the corresponding values of the efficiencies for each set of primary inlet conditions. Note that it was chosen to set $\eta_{py} = \eta_s$ as the effect of those two efficiencies on the characteristic curve is similar [110]. The primary nozzle efficiency η_p is first calibrated to get a match for the primary mass flow rate. Then the process is repeated for η_{py} and η_s to match the choked secondary mass flow rate. Finally, the mixing efficiency η_m and diffuser efficiency η_d are set to fit the off-design part of the curve. From Table 4.4, it appears that primary and secondary efficiencies (η_p , η_{py} and η_s) are decreasing as the primary pressure or temperature is increased, which reflects on the increased friction losses due to a higher

4 | Optimal ejector exergy efficiency and COP

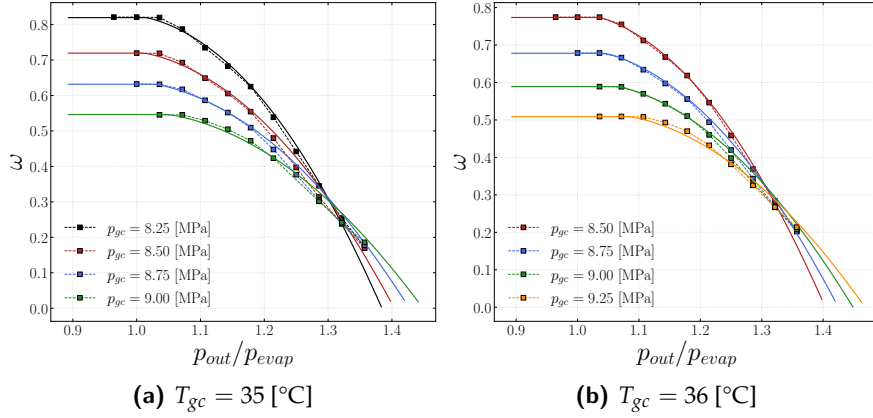


Fig. 4.6 Fitting of the characteristic curves (plain line) onto the CFD-HEM results (squares). The related fitting efficiencies are given in Table 4.4.

flow acceleration along its expansion. As for η_m , it was chosen to fix this efficiency to 0.95 as in [109]. Hence, η_d is set to properly fit the off-design part of the curves. Notice that low values of η_d were determined, which is a consequence of the limitation of the model to constant efficiencies for a same characteristic curve. In practice, all efficiencies should be modified along a same characteristic curve as p_{out} varies and correlations for the efficiencies should be found to enhance its prediction capability, but are beyond the scope of the present analysis. In addition, the thermodynamic model is only used in this study to generate a continuous operation curve and its function

T_{gc} [°C]	p_{gc} [MPa]	η_p	$\eta_{py} = \eta_s$	η_m	η_d
35	8.25	0.97	0.96	0.95	0.35
	8.50	0.97	0.96	0.95	0.28
	8.75	0.97	0.95	0.95	0.24
	9.00	0.95	0.92	0.95	0.23
36	8.50	0.97	0.96	0.95	0.32
	8.75	0.97	0.95	0.95	0.28
	9.00	0.96	0.93	0.95	0.26
	9.25	0.94	0.91	0.95	0.26

Table 4.4 Fitting efficiencies for each set of gas cooler exit temperature and pressure (Fig. 4.6).

is thus limited to fit the CFD data, which is achieved properly, as per Figure 4.6.

By combining the predictions of the calibrated ejector model and that of the cycle model, the operation curve can be determined. Since the fitting efficiencies vary with the inlet conditions, the operation curves are constructed by parts, where for each value of T_{gc} , said efficiencies are calculated by linear interpolation of the values reported in Table 4.4, as a function of p_{gc} . Above and below the calculated gas cooler pressures, the efficiencies are constant and equal those at the nearest fitted p_{gc} value (e.g., at $T_{gc} = 35$ [°C] and $p_{gc} = 8$ [MPa], the efficiencies are those obtained for $p_{gc} = 8.25$ [MPa]). Figure 4.7 shows COP maps obtained via Equation (4.9) for both supercritical inlet temperatures, where operation curves are plotted in plain green lines. The dotted green curves are the on/off-design regime limits (i.e., on-design regime on the left and off-design on the right). The location along the operation curve where the COP reaches its maximum value is highlighted by a star. In addition, the discrete positions in the diagram for which CFD computations have been performed are indicated by the squares (same colors as in Figure 4.6), for reference. Moreover, the gray portion of

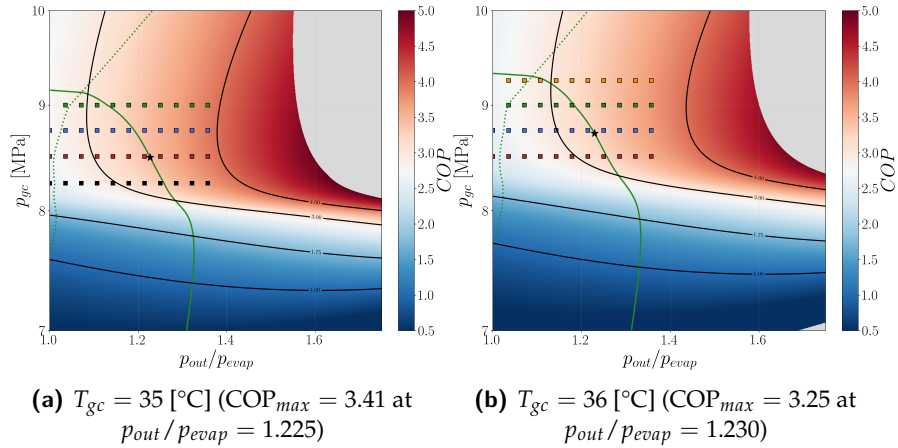


Fig. 4.7 COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio $p_{\text{out}}/p_{\text{evap}}$. Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Discrete CFD calculation points are indicated by the squares (same colors as in Figure 4.6) and the maximum COPs along the operation curves are highlighted by stars. Iso-COP lines are plotted in black.

4 | Optimal ejector exergy efficiency and COP

the diagram corresponds to a non-physical region (second principle not respected or backflow operation [111]). Confirming the previous work of Metsue *et al.* [111], the maximum COP is reached when the ejector operates under off-design. In fact, the majority of the operation curve is located within the off-design operation region. Notice that the maximum COPs are found for $p_{gc} \approx 8.5$ [MPa] and $p_{gc} \approx 8.75$ [MPa] for $T_{gc} = 35$ [°C] and $T_{gc} = 36$ [°C], respectively. The four gas cooler pressures that were selected for the analysis then indeed correspond to the pressure range in which the COP is expected to have reasonably high values.

4.4.2 Exergy transfers vs COP

As a second step, one investigates the exergy transfers from the primary to the secondary stream within the ejector by conducting an exergy tube analysis. Figures 4.8a and 4.8b show for $T_{gc} = 35$ [°C] and $p_{gc} = 8.5$ [MPa] the dimensionless cumulative transfer of total exergy $I_\xi(z)$ and exergy destruction $\Pi(z)$ along the axial direction, respectively. Four compression ratios p_{out}/p_{evap} are plotted to make the trends apparent, with $p_{out}/p_{evap} = 1.07$ corresponding to a near critical operation case. One may then notice that as the compression ratio decreases, there is a (positive) shift in the axial direction at which exergy transfers and losses within the secondary stream occur. Moreover, the trend of the curves in Figures 4.8a and 4.8b invert depending on the compression ratio near $z/L \approx 0.5$, as the exergy transfers and losses within the secondary stream occur at different axial positions of

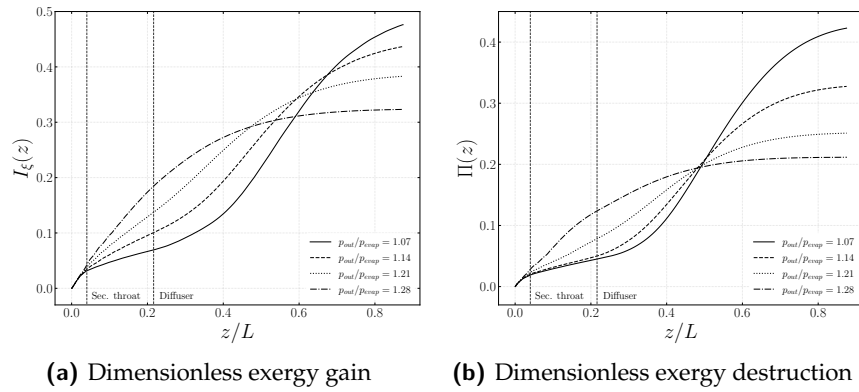


Fig. 4.8 Dimensionless exergy gain and destruction along the axial direction of the ejector (Fig. 4.5) for $T_{gc} = 35$ [°C] and $p_{gc} = 8.5$ [MPa].

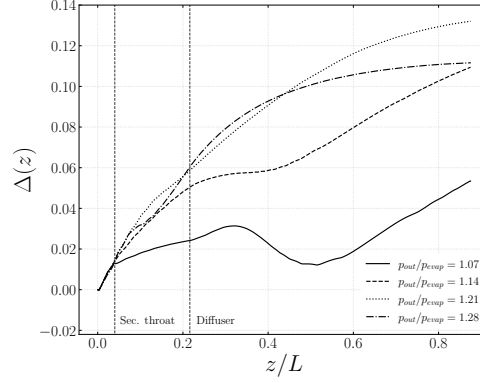


Fig. 4.9 Dimensionless net exergy gain of the secondary stream for $T_{gc} = 35$ [°C] and $p_{gc} = 8.5$ [MPa].

the ejector. For example, at a relatively low compression ratio ($p_{out}/p_{evap} = 1.07$), the exergy transfers and exergy losses within the secondary stream occur further downstream than in the case $p_{out}/p_{evap} = 1.28$. This behavior may be attributed to the increased mean velocity of the flow within the secondary throat and diffuser as the outlet pressure is lowered (i.e., lower compression ratio), hence delaying, or pushing the transfers and losses downstream. Consequently, the outlet values of I_{ξ} and Π get higher as the the compression ratio is decreased. It is then clear that there is a competition between exergy gain and destruction, and the dimensionless net exergy gain of the secondary stream may then be calculated to shed light onto this phenomenon, as shown in Figure 4.9. Interestingly, it is found that unlike reported by Lamberts *et al.* [83], the maximum Δ is not found at critical conditions, but rather under off-design regime (at $p_{out}/p_{evap} = 1.21$ in Figure 4.9).

To determine the outlet pressure that maximizes the dimensionless net outlet exergy gain of the secondary stream Δ_{out} (that is, the value of Δ at the outlet of the ejector), Figure 4.10 displays Δ_{out} as a function of the compression ratio for both considered T_{gc} values. The diamonds highlight the position of the intersection with the operation curve (green curve of Fig. 4.7). Note also that additional CFD points have been calculated to locate the maximum more accurately. For a same gas cooler pressure, the exergy gain first increases, then decreases beyond a particular compression ratio because the exergy destruction within the secondary stream decreases more slowly than the exergy gain provided by the primary stream as the

4 | Optimal ejector exergy efficiency and COP

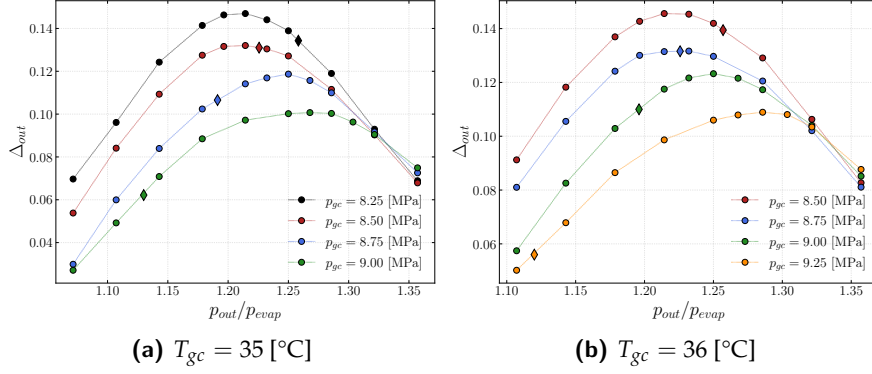


Fig. 4.10 Dimensionless net outlet exergy gains of the secondary stream Δ_{out} as a function of the compression ratio. The diamonds indicate the points of intersection with the operation curve.

compression ratio gets higher, as it can be observed by looking at the values of I_ξ and Π at the outlet in Figure 4.8. It is also apparent that as p_{gc} increases, Δ_{out} generally gets lower and its maximum is found for higher compression ratios. However, beyond a compression ratio of about 1.3, the secondary stream mass flow rates at high gas cooler pressures (e.g., $p_{gc} = 9$ [MPa]) are higher than that at lower gas cooler pressures (e.g., $p_{gc} = 8.25$ [MPa]), as visible in Figure 6. Since, as per Equation 4.7, the secondary mass flow rate is at the numerator, the related values of Δ_{out} in Figure 10 reflect on this behavior, which explains why beyond $p_{out}/p_{evap} > 1.3$, Δ_{out} at $p_{gc} = 9$ is lower than at $p_{gc} = 8.25$ [MPa]. More importantly, notice that for both T_{gc} , the intersection of Δ_{out} with the operation curve at the location of the maximum COP (e.g., at $p_{gc} \approx 8.5$ for $T_{gc} = 35$ [°C], Fig. 4.7a) is found in the near vicinity of the maximum Δ_{out} . This implies that for the presently studied cases, there is a direct correlation between local- and global-scale performances. In addition, those operation points correspond to off-design operations of the ejector, hence with non-maximum entrainment ratios. Thus, to optimize the ejector and improve the COP of the cycle, the objective function should be to maximize the dimensionless net exergy gain of the secondary stream, instead of maximizing the entrainment ratio. Note that the results are not biased by any post-process treatment, as both approaches (CFD and 0D modeling) are performed independently, and the fitting of the thermodynamic model is done, as stated in Section 4.4.1, only to calculate the cycle operation curve continuously, i.e., in between the CFD points.

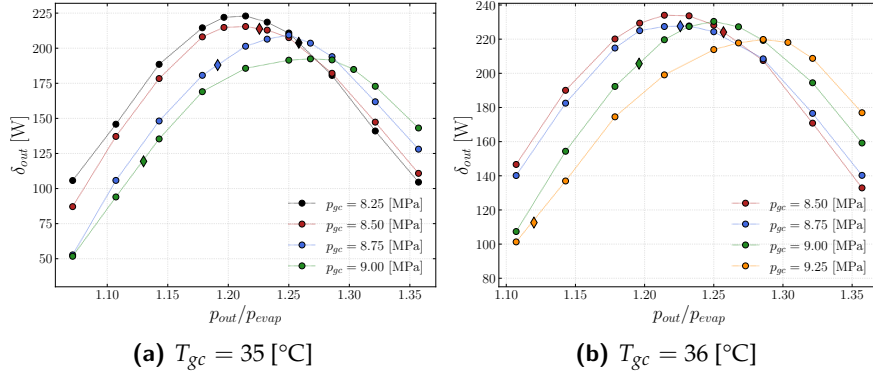


Fig. 4.11 Net outlet exergy gains of the secondary stream δ_{out} as a function of the compression ratio. The diamonds indicate the points of intersection with the operation curve.

Building on the previous observation, Figure 4.11 displays the dimensional net gain of total exergy of the secondary stream δ_{out} . It is then visible that for both T_{gc} values, the net gain of exergy at the operation points (diamonds) is the highest in the near vicinity of the maximum COP point (on the red curve at $T_{gc} = 35$ [°C] and on the blue curve at $T_{gc} = 36$ [°C]). This means that as it could be suspected, and since the secondary inlet conditions are fixed in this analysis, the maximum COP is theoretically reached when the absolute total exergy flow rate of the secondary stream is the highest at the outlet of the ejector. Indeed, even though Δ_{out} may be higher for operation at lower p_{gc} , the exergy flow of the primary stream (i.e., $\dot{m}_p \zeta_{gc}$) is lower and therefore less exergy content is transferred to the secondary stream.

4.5 Results and discussion for subcritical operations

In this section, the ERS is studied under subcritical operations to determine if the conclusions of Section 4.4 are still valid. A similar analysis is therefore conducted in Section 4.5.1. As metastability is expected for subcritical primary inlets, HRM simulation results are also compared to HEM results in Section 4.5.2.

4.5.1 Operation and exergy transfers at equilibrium

As in Section 4.4.1, CFD-HEM characteristic curves are used for calibrating the thermodynamic model at $T_{gc} = 25$ [°C] and for four values of p_{gc}

4 | Optimal ejector exergy efficiency and COP

T_{gc} [°C]	p_{gc} [MPa]	η_p	$\eta_{py} = \eta_s$	η_m	η_d
25	6.45	0.99	0.93	0.95	0.30
	6.55	0.99	0.93	0.95	0.29
	6.70	0.99	0.93	0.95	0.28
	6.95	0.99	0.93	0.95	0.26

Table 4.5 Fitting efficiencies for each gas cooler exit pressure at $T_{gc} = 25$ [°C].

indicated in Table 4.2. Table 4.5 summarizes the obtained fitting efficiencies. Note this time that only the diffuser efficiency varies to fit the simulation results, and that said efficiency tends to decrease as p_{gc} increases. It is also visible that η_p is higher than for transcritical operation (Tab. 4.4). Figure 4.12 shows the result of the calibration process, that yields significantly less accurate predictions than in the transcritical case. The angle near the critical point (on/off-design junction) could not be accurately fitted while simultaneously matching primary and secondary on-design mass flow rates (or in other words, the on-design plateau). This constitutes a limitation of the thermodynamic ejector model, and it was thus chosen not to use it to determine the operation curve, but rather to utilize the CFD characteristic curves (squares with dashed lines in Figure 4.12). Figure 4.13 then shows

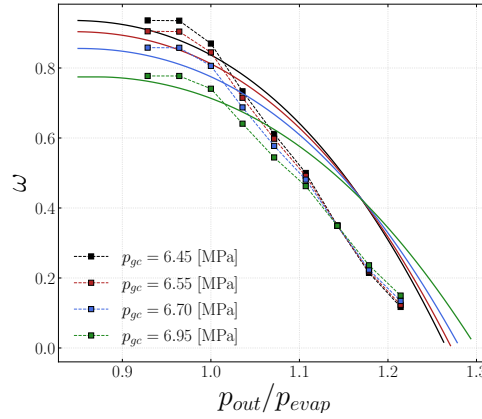


Fig. 4.12 Fitting of the characteristic curves (plain line) onto the CFD-HEM results (squares) for $T_{gc} = 25$ [°C]. The related fitting efficiencies are given in Table 4.5.

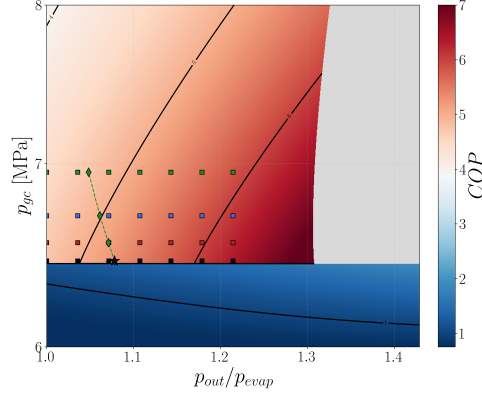


Fig. 4.13 Map of the COP as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . The partial operation curve is plotted with green diamonds and dashed line. Discrete CFD calculation points are indicated by the squares and the maximum COP along the operation curve ($COP_{max} = 5.28$ at $p_{out}/p_{evap} = 1.078$) is highlighted by the star. Iso-COP lines are plotted in black.

the COP map for $T_{gc} = 25$ [°C], with the operation points (i.e., $(p_{out} - p_{gc})$) for the four p_{gc} values considered (Tab. 4.2). One can first notice the discontinuity of the COP map at $p_{gc} = 6.44$ [MPa], which is the saturation pressure at $T_{gc} = 25$ [°C]. To illustrate why this discontinuity occurs, Figure 4.14 shows the cycle in the $p - h$ diagram as p_{gc} varies. As visible, since by construction point 3 is located on the iso-temperature ($T_{gc} = 25$ [°C]), if p_{gc} is below the saturation pressure at 25 [°C], there is no condensation, which explains the poor performance of the cycle for this operation. Hence, no CFD simulation was performed below $p_{gc} = 6.45$ [MPa]. Note that it was chosen to run the simulations at $p_{gc} = 6.45$ instead of $p_{gc} = 6.44$ (saturation pressure) to ensure the numerical robustness of the primary inlet boundary condition that is invalid for saturated states. It is then deduced from Figure 4.14 that the maximum COP is found (under the modeling hypotheses of Section 4.3.5) under saturated liquid conditions (i.e., at the location of the discontinuity). This is because as p_{gc} is increased (going from point 3 to 3⁺), the compression work ($h_2 - h_1$) is increased while the cooling effect ($h_1 - h_3$) does not vary by much, hence the COP decreases as p_{gc} increases (Eq. (4.9)). Consequently, a full operation curve is not required for the analysis as p_{gc} at the maximum COP point is known. In addition, note that the on/off-design limit is not visible in Figure 4.13 because it lies outside of

4 | Optimal ejector exergy efficiency and COP

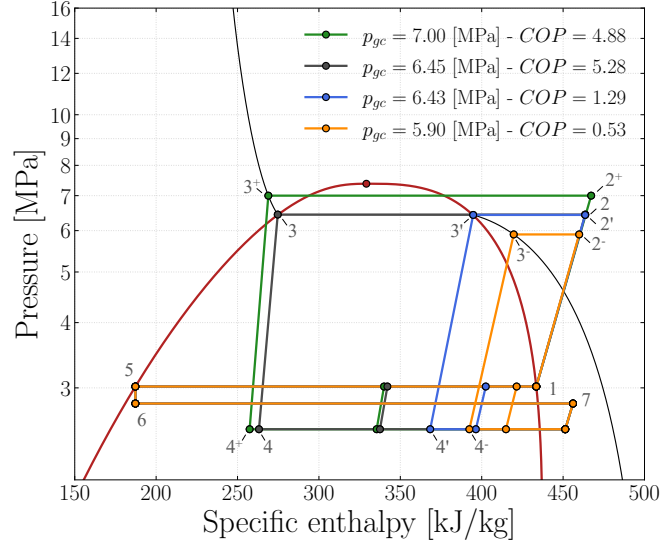


Fig. 4.14 Ejector refrigeration cycle in the $p - h$ diagram. In red: the saturation curve and critical point (dot); black line: iso-temperature $T_{gc} = 25$ [°C]. The cycle is represented for four p_{gc} values including the two limit states at the discontinuity. Point 3 is located on the iso-temperature by construction of the model.

the axes boundaries (all states are off-design).

After repeating the previous exergy analysis procedure for the subcritical case, Figure 4.15 displays Δ_{out} and δ_{out} for selected gas cooler pressures. Note that the case $p_{gc} = 6.55$ [MPa] is not shown, as this case is mostly used for the metastability analysis in the following section. As per Figure 4.15a, one can see that there is no correlation between the maximum ejector exergy efficiency and maximum COP. Indeed, the maximum COP is found near ($p_{gc} = 6.45$ [MPa] - $p_{out}/p_{evap} \approx 1.075$), which is marked by the black diamond in Figure 4.15. However, the maximum Δ_{out} and δ_{out} are found in the near vicinity of $p_{out}/p_{evap} \approx 1.125$. Nonetheless, as shown by Figure 4.15, the operation point with maximum COP (black diamond) still yields the highest net outlet exergy gain along the operating curve. Since the present ejector (Tab. 4.1) has been designed to operate at transcritical operating conditions, this illustrates that the current design is not suitable for optimal operation at subcritical operation conditions. Hence, the ejector cannot fully deliver its maximum gain to the system and is forced, by

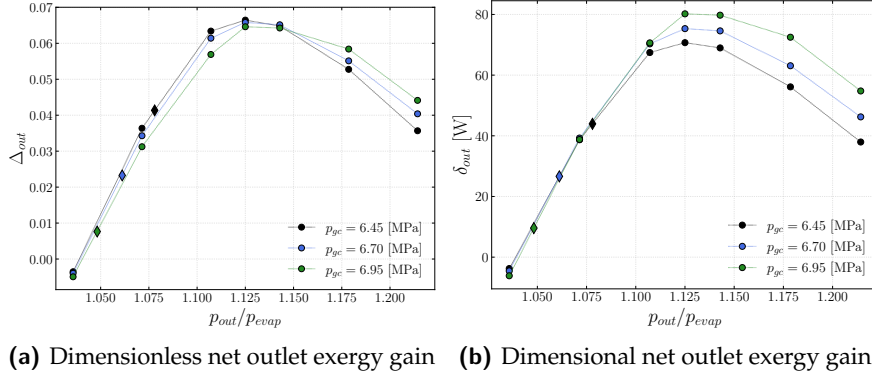


Fig. 4.15 Net outlet exergy gains of the secondary stream as a function of the compression ratio for $T_{gc} = 25$ [°C]. The diamonds indicate the point of intersection with the operation curve.

system requirements, to operate at sub-optimal conditions at the local scale, because of ejector-cycle adaptation.

4.5.2 Impact of metastability

In this section, it is proposed to study the influence of metastability on (i) the ejector characteristic curves and internal flow field, and (ii) on the global operation of the ERS. To do this, HEM and HRM are compared. For the HRM, two relaxation times are considered, that are, $\theta = 2.10^{-6}$ [s] and $\theta = 4.10^{-6}$ [s]. As reported in Metsue *et al.* [113], a relaxation time of 5.10^{-6} [s] allowed for the best matching of the CO₂ nozzle outlet pressure. However, such a value could not be used with the present ejector as the spinodal limit (i.e., the limit beyond which the fluid becomes unstable) would be reached. This is likely because the present primary nozzle diverging angle is significantly higher than in the case of [113], and the quality gradients are consequently higher. In addition, the analysis in this section is performed at $p_{gc} = 6.55$ [MPa] instead of 6.45 [MPa] which would have been too close to the saturation conditions at the inlet boundary. This would induce flashing right at the primary nozzle inlet, which is not handled by the boundary conditions.

Figure 4.16a shows the primary/secondary mass flow rates obtained using the HEM and HRM at $T_{gc} = 25$ [°C]. As expected, the HRM predicts higher primary mass flow rates than the HEM, with about a 5.5% and 10.4% increase for $\theta = 2.10^{-6}$ [s] and $\theta = 4.10^{-6}$ [s], respectively. Indeed, as

4 | Optimal ejector exergy efficiency and COP

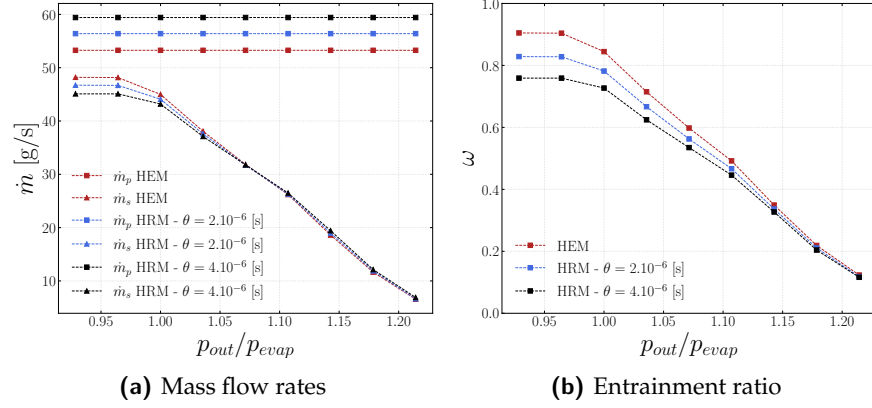


Fig. 4.16 Primary/secondary mass flow rates and entrainment ratios using the HEM and HRM ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]).

pointed out by De Lorenzo [40], adding non-equilibrium effects increases the speed of sound of a two-phase mixture, which then increases the critical mass flow rate (at choking conditions). The HEM thus provides the lowest achievable bound of choked mass flow rate in a nozzle. As for the secondary

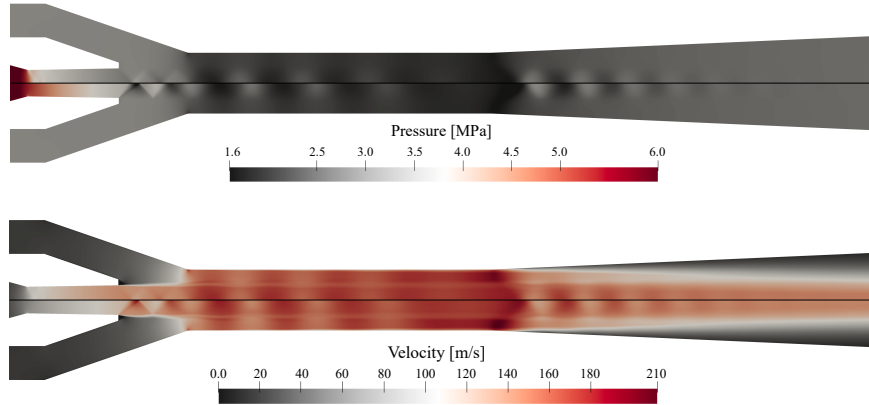


Fig. 4.17 Pressure and axial velocity contours obtained using the HEM (top half) and HRM with $\theta = 4.10^{-6}$ [s] (bottom half) (zoom on the relevant portion of the ejector). Results for $p_{gc} = 6.55$ [MPa], $T_{gc} = 25$ [°C] and $p_{out}/p_{evap} = 0.96$.

flow, it is noticed that there is only a slight deviation between HEM and HRM under the off-design regime, but a visible decrease under near-critical and on-design operations. Figure 4.16b then displays the corresponding characteristic curves. The metastability tends to decrease the performance (in the sense of entrainment ratio) of the ejector. In fact, as visible in Figure 4.17, where the pressure and axial velocity contours are shown for HEM and HRM with $\theta = 4.10^{-6}$ [s] at $p_{out}/p_{evap} = 0.96$, the pressure at the primary nozzle exit is higher for the HRM case. Consequently, the shock train within the mixing chamber and constant area duct is stronger since the nozzle is more under-expanded than predicted by the HEM, as it is clearly visible on the axial velocity profile. Then, as the primary stream expands more into the mixing chamber, the secondary stream section area is reduced, thereby decreasing the secondary mass flow rate.

As a last step of the present work, the exergy analysis is performed on HRM cases to shed light onto how the exergy transfer phenomena are affected by the presence of the metastable phase. Figure 4.18 shows the dimensionless exergy gain and destruction along the axial direction of the ejector in HEM and HRM with $\theta = 4.10^{-6}$ [s] and for two compression ratios ($p_{out}/p_{evap} = 0.96$ is on-design and $p_{out}/p_{evap} = 1.11$ is off-design). I_ξ and Π are about 8% lower with the HRM than with the HEM. In other words, the metastability introduced into the primary nozzle effectively decreases the exergy destruction within the secondary stream, but the exergy transfer towards the secondary stream is also reduced. The profile of the

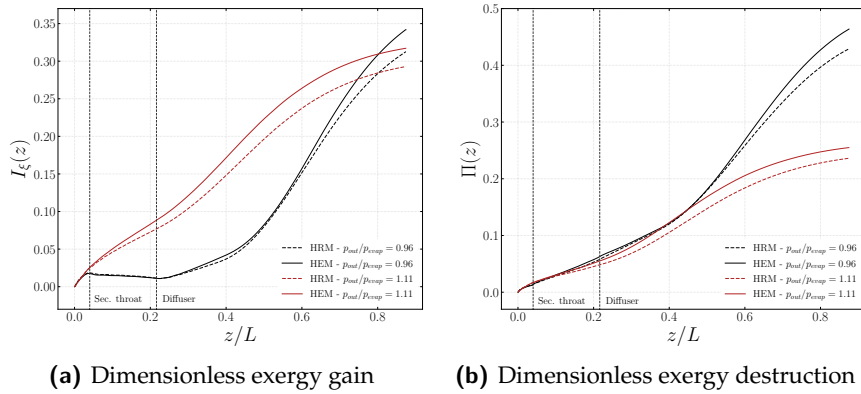


Fig. 4.18 Dimensionless exergy gain and destruction terms for $\theta = 4.10^{-6}$ [s] ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]).

4 | Optimal ejector exergy efficiency and COP

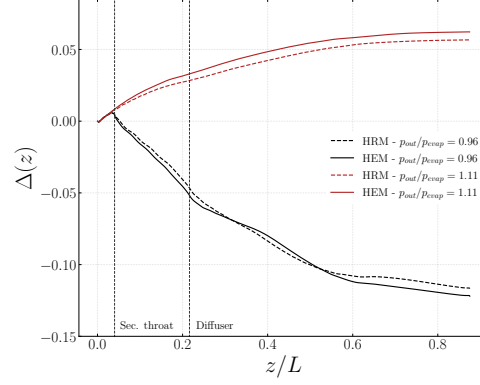
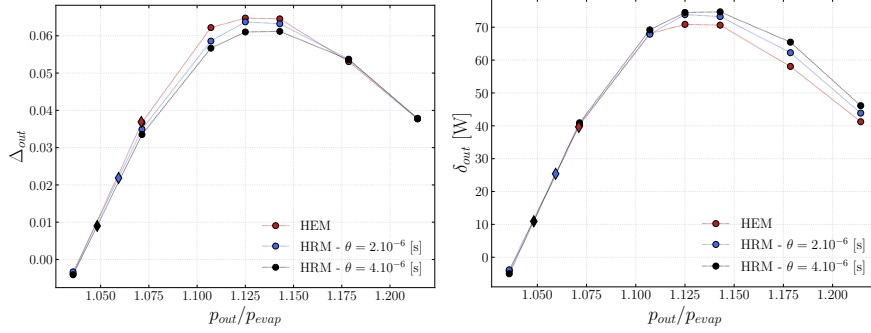


Fig. 4.19 Dimensionless net exergy gain of the secondary stream in HEM and HRM with $\theta = 4.10^{-6}$ [s] ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]).

dimensionless net exergy gain, as displayed in Figure 4.19, is again determined by the competition of the gains and losses of the secondary stream. The Δ -HRM for the off-design case is lower than its Δ -HEM counterpart whereas the opposite observation is made for the on-design case. This is because for the on-design case, the secondary stream outlet total exergy is negative. However, the dimensional net exergy gain profiles δ -HRM are indeed systematically lower than the δ -HEM ones. This behavior may mostly be attributed to the higher primary mass flow rate (at the denominator of Equations (4.5)-(4.7)). Overall, this indicates a lesser performance of the ejector as thermodynamic non-equilibrium effects are introduced into the modeling approach. To determine the physical (local) mechanisms leading to this decreased ejector performance, a deep analysis of different sources of exergy transfers and destruction terms should be conducted on both primary and secondary streams. However, this goes beyond the scope of the present work and should require additional tools such as large eddy simulation (LES) in order to shed light onto the real physics including fluctuations/fluxes and then the transport of turbulent quantities. As a final step, it is then proposed to analyze Figure 4.20, that shows dimensionless and dimensional net outlet exergy gains of the secondary stream, comparing HEM and HRM results. Despite Δ_{out} showing lower values as the relaxation time increases (larger metastability effects), one may see that δ_{out} is conversely getting higher, for a same compression ratio. Again, this may mostly be attributed to the higher mass flow rate in HRM, thereby carrying



(a) Dimensionless net outlet exergy gain (b) Dimensional net outlet exergy gain

Fig. 4.20 Net outlet exergy gains of the secondary stream as a function of the compression ratio with the HEM and HRM ($p_{gc} = 6.55$ [MPa] and $T_{gc} = 25$ [°C]). The diamonds indicate the point of intersection with the operation curve.

more exergetic content. On the other hand, the operation point (diamond) gets severely affected by metastability, as both Δ_{out} and δ_{out} get significantly lower, recording more than a 70% decrease of δ_{out} between HEM and HRM with $\theta = 4.10^{-6}$ [s]. Lastly, one can compare the COP that could be obtained from the predictions of the HRM to that of the HEM, which shows that the operation point deduced from the prediction of the HRM (with $\theta = 4.10^{-6}$ [s]) yields $COP = 5.01$, compared to that predicted by the HEM with $COP = 5.16$. From the analysis, it is evident that despite increasing the primary mass flow rate of the ejector, the metastability mostly accounts for decreased performance of both the ejector and the ERS. This implies that performing simulations in HEM does not provide conservative results but rather optimistic ones compared to the reality, which highlights again the need for numerical algorithms that account for metastable phenomena.

4.6 Conclusions

In this work, a multi-scale approach to study the exergy transfers within transcritical and subcritical CO_2 ejectors and their impact on the global performance of an ERS was presented. On the CFD scale, the density-based SU2 solver was utilized to perform wall-resolved simulations of the ejector, enabling the access to the local flow fields. At the system scale, the thermodynamic ejector model of Metsue et al. [110] was calibrated onto the

CFD results and integrated into the 0D model of a typical CO₂ ERS.

Firstly, the analysis under transcritical operation showed that for fixed inlets conditions, there exists a compression ratio that maximizes the net exergy gain of the secondary stream, which is likely to be found under off-design regime. In addition, it was found that at the point of maximum COP that could theoretically be obtained (according to the operation curve), the dimensionless net exergy gain of the secondary stream is maximum along a fixed primary inlet pressure (i.e., along the same characteristic curve). This means that there is a direct correlation between ejector and cycle performances. Further analysis then demonstrated that the point of maximum COP had the overall maximum –dimensional– net exergy gain along the operation curve.

Secondly, the analysis under subcritical operation showed that the maximum net exergy gain remained maximum at the optimal COP operating point, but that said point did not correspond to a maximum along the same characteristic curve. This is attributed to the fact that the ejector geometry used for the analysis was not intended for subcritical operation conditions. Thus, the ejector could not deliver its full capabilities as a results of its integration into a non suitable cycle. Then, the HRM was used to highlight the effects of metastability on the performance of the ejector and that of the ERS. As the relaxation time of the HRM increases (i.e. accentuating non-equilibrium effects), the ejector performance globally decreases, both in terms of entrainment ratio and exergy transfers. Indeed, using a typical relaxation time with the HRM showed that a more than 70% decrease of net exergy gain could be expected compared to the predictions of the HEM, which translated to a COP decrease of about 3%. This illustrates that HEM calculations are not conservatives.

It is important to keep in mind that the two approaches used for the present discussion (CFD and 0D modeling) are independent of each other. It is also worth noting that although there is an evident correlation between the performance at the local and global scales, there is no analytical proof that can demonstrate this. Therefore, future work may be performed for an increased number of operating conditions and for different ERS configurations. It is also the authors' opinion that a proper validation of the present deductions will only be possible when compared to high quality (CFD grade) experimental measurements, even possibly with local flow measurements and/or visualizations, also to shed light onto the occurrence and importance of thermodynamic non-equilibrium effects. Lastly, the analysis of high fidelity numerical simulations are foreseen as the FANS

simulations may not account for complex turbulent phenomena (turbulent fluxes through the dividing streamline) that, at some level, dictate part of the exergy transfers and losses within the ejector [35].

5

Conclusions

Predicting the performance of two-phase CO₂ ejectors presents a significant challenge due to the requirement of advanced modeling techniques and the limited availability of validation data at the time of the present research. Numerical methods are a precious tool to study the local flow characteristics of the device, but the accuracy of two-phase simulations is lagging behind what is currently possible in single-phase. Consequently, the design of ejectors for refrigeration systems remains difficult, which limits their implementation in commercial systems. In this context, the present work contributed to partially catching up with the maturity level that has already been acquired in single-phase ejectors.

The study focused on the open-source density-based SU2 solver to perform CFD and have access to the local flow features. The solver has been modified to make it compatible with two-phase CO₂ by the coupling of a tabulated EoS. The latter was implemented from scratch as a Python routine to generate and store the tables in pre-processing, which are accessed by SU2 through a C++ routine. Additionally, a HRM was implemented directly within SU2 to study the influence of metastability. Thermodynamic modeling was used to determine the operation of the ERS, with a calibrated ejector model that allowed the prediction of ejector performance under all modes. The combination of the CFD and thermodynamic modeling tools enabled to partially bridge the gap between local behavior at the ejector level and the global performance of the ERS.

5.1 Specific achievements

Through the implementation of the aforementioned novel simulation tools and the extension of existing post-processing methods to the particular case of two-phase CO_2 , this work has allowed to address some of the recent concerns with regards to the performance prediction and operation of ejector devices to be integrated into refrigeration systems. In this section, the particular achievements of the present doctoral research project are discussed.

5.1.1 Modification and implementation of CFD tools

Because the EoS constitutes the bottleneck of two-phase CFD in terms of CPU time, a fast and general method for constructing and interpolating the EoS was described. The method, based on bi-cubic functions and a quadtree algorithm with local refinement of the interpolation grid in the thermodynamic state-space, allows for reasonable storage size of tabulated properties and fast interpolation speed during CFD simulations. Although applied in the context of CO_2 in this study, the method can be universally applied to generate tables linking three thermodynamic properties for any fluid, given that the relations are obtainable from an external source, such as the REFPROP and COOLPROP libraries. Hence, the algorithm could readily be utilized to generate the interpolation tables for other fluids without the need for additional coding. The table generation method, based on an absolute error tolerance that is specified by the user for each property, ensures that the interpolation error is below the required threshold. For each thermodynamic relation, a table of roughly 100 000 points is created, requiring between 20 and 40 MB of storage. At the beginning of the CFD simulation, each table is read and stored in the RAM using a dedicated routine directly implemented into SU2. Compared to an older generation tabulated EoS algorithm [56], reported to perform about 66 times faster than the original SW EoS, the present EoS was found to yield an average solver iteration time between 2 and 6 times lower, depending on the number of processors.

As the Navier-Stokes equations are implemented in a general formulation within SU2 (no assumptions are made with regards to the EoS), simulations using the HEM could be conducted after coupling the EoS to the solver. In addition, characteristic-based (non-reflective) boundary conditions are readily available in the solver, ensuring that spurious reflection waves do

not interfere with the convergence of the solution. Using the HEM, it was found that CFL numbers up to 50 could be used with the implicit Euler time integration scheme, significantly reducing the computation time required to obtain a converged solution compared to explicit solvers, that are limited to CFL numbers below unity due to stability constraints.

A density-based formulation of the HRM was implemented for the first time in a CFD framework, and the impact of the relaxation time was studied using both constant values and a correlation [8]. HRM and HEM wall-resolved simulation results were compared to experimental flashing CO₂ nozzle pressure profiles [117]. Mass flow rates increased with the relaxation time, being notably more than 18% higher using a relaxation time that best fitted pressure profiles near the throat. This increased mass flow rate is the result of two competing phenomena: metastability reduces the flow velocity but increases the density at the choking location. Pressure and quality profiles within the device exhibited consistent behaviors when the relaxation time was increased, in agreement with current literature: rising the constant relaxation time shifts nozzle pressure profiles upward downstream of the flashing onset location and smooths the quality profiles, effectively delaying the flashing process. Increasing the relaxation time also yielded a better pressure fitting in the first half of the diffuser, however coming at the cost of an over-prediction in the second half, where lower relaxation times were preferred. The analysis suggested that metastability effects in HRM primarily occur near the throat. Consequently, the poorer pressure fitting in the second half of the diffuser can be attributed to the delay experienced in the first half of the diffuser due to these metastability effects. The correlation of Angielczyk *et al.* [8] yielded poor results, with no significant mass flow rate increase, which may indicate that relaxation time correlations are highly case-dependent on geometry and operating parameters.

5.1.2 ERS thermodynamic modeling

A theoretical analysis of a classical ERS operation was performed using a thermodynamic modeling approach. The model was implemented in Python and based on simple hypotheses regarding the cycle, such as adiabatic/isentropic transformations and saturated vapor conditions at the evaporator outlet. The evaporator temperature was fixed to -6 [°C] and three gas cooler temperatures were studied (25, 35, and 45 [°C]), with all other cycle operation parameters fixed except for the gas cooler and ejector

5 | Conclusions

outlet pressures. For the ejector, the thermodynamic model (Appendix C), integrating the real physics of the compound-choking to predict the double-choking regime, was fitted through 5 efficiencies onto two-phase CO₂ experimental mass flow rate measurements.

It was discovered that an operation curve exists, constituted by the set of operating conditions that allow steady-state operation of the ERS. This implies that, with all other parameters being set by the application, the cycle cannot operate at arbitrary gas cooler and ejector outlet pressures. The allowable pressure sets are determined by the cycle requirements and the internal physics of the ejector. Additionally, it was observed that for an ejector with realistic entropy generation associated with irreversible mixing phenomena, the maximum COP operation point tends to occur when the ejector operates in an off-design regime. As the ambient temperature increases, the optimal operation point approaches on-design ejector operation and can eventually shift to full on-design operation if the heat rejection temperature goes over a certain threshold.

It was established that the primary design strategy for the ejector within the ERS is to minimize entropy generation within the device. A reduction in any of the thermodynamic model efficiencies correlated with a decrease in the maximum achievable COP of the ERS. Furthermore, as entropy generation diminishes within the ejector, the maximum COP operation point approaches critical ejector operation conditions. Additionally, the analysis suggested that there is no benefit in operating the ejector under a full on-design regime for refrigeration applications. Optimizing the throat area ratio of the ejector only marginally improved the COP. However, it is expected that ejector dimensions directly influence the cycle performance as the cooling power deviates from design conditions due to changes in the ambient temperature.

5.1.3 Multi-scale analysis of the ejector within the ERS

A multi-scale approach was introduced to examine exergy transfers within transcritical and subcritical CO₂ ejectors and their influence on the global performance of an ERS. To this end, previously implemented tools and approaches (Sections 5.1.1 and 5.1.2) were combined. Wall-resolved simulations of the ejector were conducted using the SU2 solver at the CFD level, providing access to local flow quantities. The exergy analysis was based on the exergy tube method [83], for the first time successfully applied to two-phase CO₂ ejectors. At the system scale, the thermodynamic

ejector model [110] was calibrated on CFD results and integrated into the thermodynamic model of a typical CO₂ ERS. The operation curve of the cycle was then obtained within the COP map for fixed secondary conditions and primary inlet temperature, aiming to identify a correlation between the maximum achievable COP and optimal exergy transfers at the ejector scale. Furthermore, the effects of the metastable phase were examined under the subcritical operating regime at both scales.

Under transcritical operation, it was observed that when the theoretical maximum COP point obtainable along the operation curve was reached, so was the maximum dimensionless net outlet exergy gain of the secondary stream (Appendix B), which can be seen as a measure of the exergy transfer efficiency within the ejector. Additionally, the analysis revealed that the compression ratio that maximizes the net exergy gain of the secondary stream along a same characteristic curve is likely found under the off-design regime, unlike reported for air ejectors, where the maximum was found closer to critical operating conditions [83]. Adding to the fact that the high COPs are found for off-design operations of the ejector, this can indicate that from the perspective of the cycle, it may be preferable to have a higher compression ratio rather than maximizing the mass flow rate at the evaporator.

Under subcritical operation, the maximum net exergy gain remained highest at the maximum COP operating point. However, this point did not correspond to a maximum along the same characteristic curve, which may be attributed to the ejector geometry used in the analysis being unsuitable for subcritical operating conditions. Consequently, the ejector could not perform to its full potential because it was integrated into an inappropriate cycle. Then, the HRM was employed to shed light on the effects of metastability on ejector and ERS performance. It was discovered that as the relaxation time of the HRM increased (i.e., accentuating the effect of metastability), the global performance of the ejector decreased in terms of entrainment ratio and exergy transfers. Specifically, using a typical relaxation time for the studied operating conditions with the HRM resulted in a more than 70% decrease in net exergy gain compared to predictions of the HEM, corresponding to a COP decrease of about 3%.

5.2 Research perspectives

This final section discusses the limitations of the research and provides pathways for future work. Through this contribution, progress has been made

5 | Conclusions

toward efficient modeling of two-phase CO₂ ejectors and their operation within the ERS. However, work remains to be done in order to provide widely accessible, accurate, and fast design tools. It is the author's opinion that further progress should be made by combining findings at different scales:

- Ejector thermodynamic modeling remains the primary tool to be used for preliminary design, which is why it is important to keep improving it. There are two main ways to do this: (i) to gain a better understanding of the internal flow mechanisms depending on the operating conditions, leading to better modeling assumptions; and (ii) to develop methods to accurately calibrate the fitting coefficients of such models. However, it is clear that having access to local 2D/3D flow quantities and accurate mass flow rate predictions/measurements through CFD or experiments is a prerequisite to conduct this work, hence the need for the enhancement of those methods as well. Then, one may use the local flow fields to define flow feature laws and adapt the 0D model depending on the operation of the device (e.g., Fabri-choking vs. compound-choking). Additionally, correlations for the fitting parameters could be deduced using machine learning techniques.
- Thermodynamic ejector models should be used as part of an ERS model to study the interactions of the ejector with the other components. Dedicated software, such as Dymola, could thus be used to model an ERS with more precision, but this requires a full knowledge of all component specifications and an array of measurements for a proper calibration of such a model. This highlights once again the dire need to have access to a dedicated experimental test bench with adequate measurements. One could then go further and conduct parametric analyses of the whole ERS to construct operation maps of the cycle depending on many parameters (such as ejector geometry, size, ambient conditions, etc.), or explore unsteady operations of the ERS.
- FANS modeling remains the most affordable way to have access to local flow variables and refine the design of the ejector. Since this work contributed to implementing tools to lower the computational resources required for the simulation of two-phase CO₂ compressible flows, full 3D simulations are now accessible and should be compared

to previous 2D results to quantify the part of the physics that is missed. It should also be foreseen to implement more advanced mixture models to better account for the presence of the metastable phase, which could be activated depending on the operating conditions. However, this could only be done, again, by first gaining some insight from experiments, and those advances are thus limited by the availability of reliable experimental measurements/visualization techniques. Additionally, at the time of writing the present thesis, DNS is not achievable due to limited computational resources, and LES is at an early stage. However, high-fidelity CFD is also required as a means to obtain detailed information about the unsteady behavior of the flow and validate turbulence models in FANS. To this end, future work should be done to modify a LES solver to handle two-phase CO₂, as it was done for FANS.

- Ejector design should not be performed by considering solely the local component scale but should in some way account for the system in which it operates. Hence, it should be foreseen to define and implement an automated design method for the design of CO₂ ejectors that integrates the different tools (at the different scales) that have been developed/enhanced within the present work, essentially by building an optimization loop. Starting from a known requirement of a refrigeration system, thermodynamic modeling could be used to determine the geometry and operating parameters of the ejector; CFD simulations could then be performed, using the HEM, HRM, or even an alternative mixture model depending on the forecast operation of the cycle model, to better calibrate the thermodynamic model.
- As implied previously, the lack of experimental data can be considered the main limiting factor for progress in ejector modeling/design. It should be foreseen to work on an ERS test bench, allowing the operation of the ejector under all modes and ideally including an access to visualize the internal flow topology, either through direct visualization, shadowgraphy, Schlieren techniques, or even designing a PIV setup. From the data gathered through the experiment, all previously discussed numerical modeling techniques could be improved.



List of Publications

The following journal and conference articles have been produced during the time frame of the Ph.D. thesis:

- A. Metsue, H. Nesreddine, J. Bodys, S. Poncet, and Y. Bartosiewicz. Analysis of the exergy transfers in subcritical and transcritical CO₂ ejectors and their connection with the performance of the refrigeration cycle. Minor revision, *Energy*, 2024.
- A. Metsue, H. Nesreddine, Y. Bartosiewicz, and S. Poncet. Theoretical analysis of the optimal ejector operation and design within an ejector-based refrigeration system. Minor revision, *International Journal of Refrigeration*, 2024.
- R. Oberti, A. Metsue, Y. Fang, and S. Poncet. Numerical simulations and local entropy generation in a two-phase transcritical carbon dioxide Ranque-Hilsch vortex tube. *International Journal of Heat and Mass Transfer*, 226:125461, 2024.
- A. Metsue, S. Poncet, and Y. Bartosiewicz. A homogeneous relaxation model algorithm in density-based formulation with novel tabulated method for the modeling of CO₂ flashing nozzles. *International Journal of Refrigeration*, 161:188–201, 2024.

A | List of Publications

- A. Metsue, R. Debroeyer, S. Poncet, and Y. Bartosiewicz. An improved thermodynamic model for supersonic real-gas ejectors using the compound-choking theory. *Energy*, 238:121856, 2022.
- S. Croquer, Y. Fang, A. Metsue, Y. Bartosiewicz, and S. Poncet. Compound-choking theory for supersonic ejectors working with real gas. *Energy*, 227:120396, 2021.
- A. Metsue, H. Nesreddine, S. Poncet, and Y. Bartosiewicz. Theoretical Analysis of the Optimal Ejector Operation Within the Classical Ejector Refrigeration System. In *Proc. of the 16th IIR Gustav Lorentzen Conference on Natural Refrigerants*. College Park, USA, 2024.
- R. Oberti, A. Metsue, Y. Fang, and S. Poncet, Turbulent two-phase flows in a transcritical CO₂ Ranque–Hilsch vortex tube. In *Proc. of the 13th Turbulence and Shear Flow Phenomena Symposium*, Montreal, Canada, 2024.
- A. Metsue, H. Nesreddine, D. Monney, Y. Bartosiewicz, and S. Poncet. Simulation and exergy analysis of transcritical CO₂ ejectors flows using the implicit real gas SU2 solver. In *Proc. of the 26th IIR International Congress of Refrigeration*. Paris, France, 2023.
- A. Metsue, Y. Bartosiewicz, and S. Poncet. A fast tabulated equation of state for CFD simulation of two-phase flows. In *Proc. of the Canadian Society for Mechanical Engineering / CFDCanada 2023 International Congress*, Sherbrooke, Canada, 2023.
- R. Oberti, A. Metsue, Y. Fang, J. Lagrandeur, S. Poncet, and D. Monney. Numerical simulation of a two-phase transcritical CO₂ Ranque–Hilsch vortex tube. In *Proc. of the 26th International Congress of Refrigeration*, Paris, France 2023.
- C. P. Rand, A. Metsue, M. Poirier, S. Poncet. Waste heat recovery of industrial exhaust gas : study of variable power ejector cooling systems. In *Proc. of the Canadian Society for Mechanical Engineering / CFDCanada 2023 International Congress*, Sherbrooke, Canada, 2023.
- A. Metsue, R. Debroeyer, S. Poncet, and Y. Bartosiewicz. An improved thermodynamic model for supersonic ejectors. In *Proc. of the the Heat Powered Cycles conference*, Bilbao, Spain, 2021.

- A. Metsue, Y. Bartosiewicz, and S. Poncet. Investigation on ejector design for CO₂ heat pump applications using Dymola. In *Proc. of the 9th IIR International Conference Ammonia and CO₂ Refrigeration Technologies*, VC, 2021.
- S. Croquer, A. Metsue, Y. Fang, Y. Bartosiewicz, and S. Poncet. Choking behavior in real-gas supersonic ejectors using compound flow theory. In *Proc. of the 15th Int. Conf. Heat Transfer, Fluid Mech. & Thermodynamics (HEFAT)*, VC, 2021.

B

Complementary Analyses on Net Outlet Exergy Gains and COP Improvement Compared to the Basic Four-Components Cycle

In this Chapter, additional analyses regarding the content of Chapter 4 are presented. Those results are presented separately in this appendix because they could not be integrated to the related article (Chapter 4) prior to publication.

2.1 Exergy gains required by the cycle

Since all cycle parameters can be deduced from the cycle requirements (Table 3.1), the dimensionless net outlet exergy gain of the secondary stream, Δ_{out} , can be fully defined from the thermodynamic modeling solely. Note however that the CFD data are still required to determine the performance of the ejector in terms of entrainment ratio, and hence to determine the operation curve. In addition, the dimensional net outlet exergy gain, δ_{out} , can be defined from the cycle requirements and a prediction of primary mass flow rate, since $\delta_{out} = \dot{m}_p \xi_{t,gc} \Delta_{out}$. It is then proposed to add iso-net outlet exergy gain lines to the results of Figure 4.7. The modified COP maps are shown for $T_{gc} = 35$ [°C] and $T_{gc} = 36$ [°C] in Figure B.1, where iso- Δ_{out}

B | Complementary Analyses

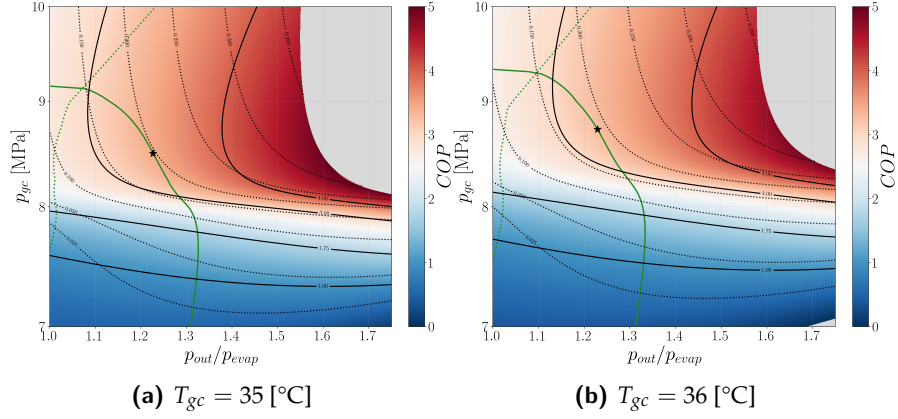


Fig. B.1 COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP and iso- Δ_{out} are plotted in plain black and dotted black, respectively. The maximum COP (also maximum Δ_{out}) along the operation curve is highlighted by the star.

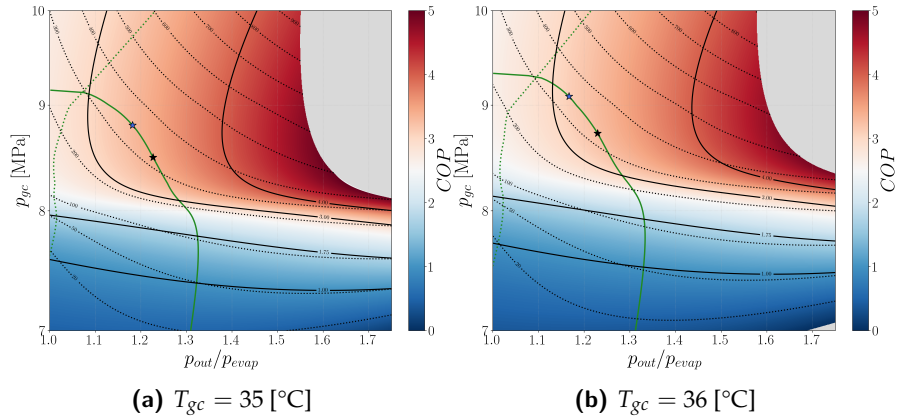


Fig. B.2 COP maps as a function of the gas cooler pressure p_{gc} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP and iso- δ_{out} (in [W]) are plotted in plain black and dotted black, respectively. The maximum COP and maximum δ_{out} along the operation curve are highlighted by the black and blue stars, respectively.

lines are added, and Figure B.2, where iso- δ_{out} are added. Note that the primary mass flow rate to compute δ_{out} in Figure B.2 is predicted using the calibrated thermodynamic model (Section 4.4.1).

First, it is visible in Figure B.1 that the maximum Δ_{out} along the operation curve occurs, this time, at the point of maximum COP (highlighted by the star). However, the point of maximum δ_{out} along the operation curve is also changed (it is found at higher gas cooler pressures), and was highlighted by the blue star in Figure B.2. Although the conclusions that may be drawn from those results are somewhat different from the original ones, presented in Chapter 4, there remains a clear correlation between the maximum achievable COP within the cycle and the exergy efficiency at the ejector scale. In other words, this time, the correlation is found through Δ_{out} and not δ_{out} , which is actually a more natural correlation since Δ_{out} is a measure of the exergy transfer efficiency, whereas $\delta_{out} = \dot{m}_s \zeta_{s,out}$ (Eq. 4.7) is rather a measure of the exergy content of the secondary stream.

Figure B.3 shows the profiles of Δ_{out} and δ_{out} obtained from the CFD at the ejector outlet and the value imposed by cycle requirements along the operation curve (here, as a function of p_{gc}), for $T_{gc} = 35$ [°C] and $T_{gc} = 36$ [°C]. As visible, there is a large discrepancy between ejector outlet and cycle requirements values. The discrepancy can be attributed to the fact that primary and secondary streams are generally not fully mixed at the ejector

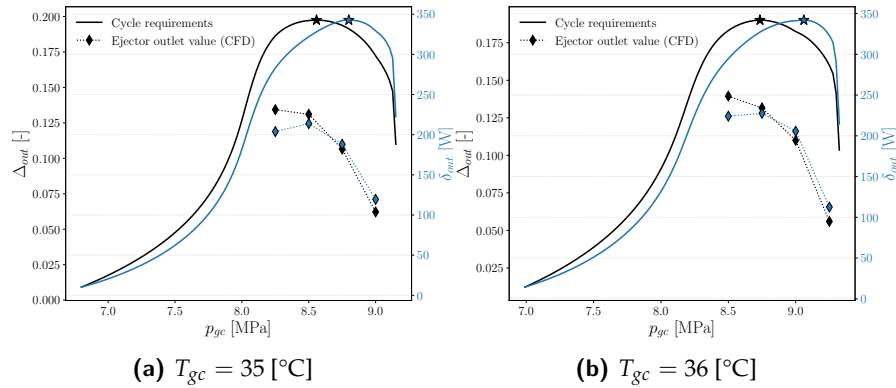


Fig. B.3 Dimensional (black) and dimensionless (blue) net exergy gains obtained from cycle requirements and values obtained at the ejector outlet. The stars indicate the maximum of the cycle requirements curves. Results are obtained for two gas cooler temperatures: (a) $T_{gc} = 35$ [°C] and (b) $T_{gc} = 36$ [°C].

B | Complementary Analyses

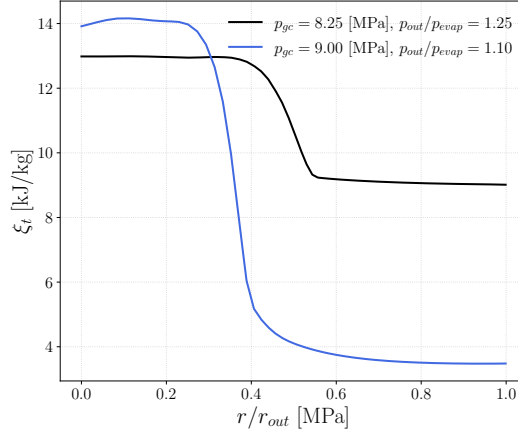


Fig. B.4 Total specific exergy profile at the outlet of the ejector along the radial direction at two different operation points ($T_{gc} = 35$ [°C]). The radial coordinate is r and the diffuser outlet radius is r_{out} .

outlet, depending on the operation conditions. This discrepancy increases with the gas cooler pressure, but this phenomenon actually depends on both the gas cooler pressure and also the compression ratio (i.e., the compression ratio generally decreases as p_{gc} increases along the operation curve, as visible in Figure B.1). To illustrate that point, Figure B.4 compares the profiles of the total specific exergy along the radial direction at the ejector outlet obtained with the CFD solver for two operation points. Those points correspond to those shown in Figure B.3a at $p_{gc} = 8.25$ [MPa] (lower discrepancy) and $p_{gc} = 9.00$ [MPa] (higher discrepancy). Indeed, the radial total specific exergy profile at $p_{gc} = 9.00$ [MPa] is less uniform than at $p_{gc} = 8.25$ [MPa], hence the two streams are less (relatively) well mixed at the ejector outlet. Note that, in practice, the flow should continue mixing within the piping connecting the ejector outlet to the separator, so that the flow entering the latter component is indeed well mixed. In the present case, the CFD results might also indicate that the ejector was not (well) designed to operate at the particular sets of operating conditions simulated in the present work.

Figure B.5 shows the COP maps with iso- Δ_{out} and iso- δ_{out} lines at $T_{cond} = 25$ [°C]. Note that since this case corresponds to a subcritical operation of the ERS, a condenser should be used, in practice, instead of a gas cooler. To reflect on this, p_{cond} is substituted to p_{gc} . As explained in Chapter 4, the

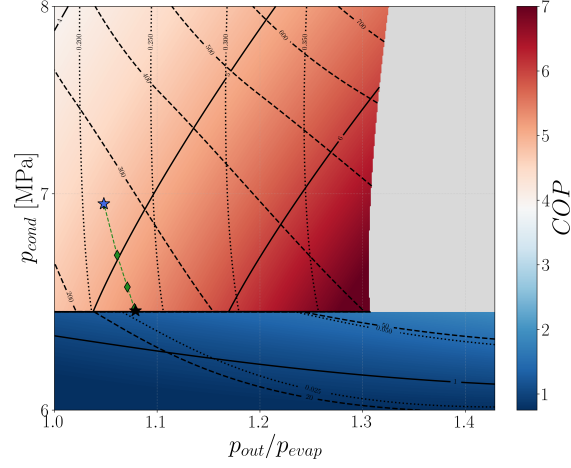


Fig. B.5 COP maps as a function of the condenser pressure p_{cond} and the compression ratio p_{out}/p_{evap} at $T_{gc} = 25$ [°C]. The operation curve is plotted in green (diamonds and dashed line), iso-COPs are plotted in plain black, and iso- Δ_{out} and iso- δ_{out} are plotted in dashed and dotted black, respectively. The maximum COP and maximum δ_{out} along the operation curve are highlighted by the black and blue stars, respectively.

fitting of the thermodynamic model onto the CFD results is unsatisfactory, hence a continuous operation curve cannot be reconstructed and the partial curve obtained via discrete CFD points is plotted instead. Much as in the transcritical case, the maximum Δ_{out} is found at the maximum COP point and the maximum δ_{out} is found at higher values of p_{cond} .

2.2 COP improvement compared to the basic four-components cycle

As mentioned in Chapter 1, the addition of the ejector within the cycle is intended to improve the COP of the classical four-components refrigeration cycle (Fig. B.6). The COP maps presented in Section 4.4.1 are this time expressed in terms of COP improvement ratio (ratio of the ejector cycle COP (COP_{ej}) to the basic cycle COP (COP_{basic})) in Figure B.7 for transcritical operation and in Figure B.8 for subcritical operation. The same gas cooler and evaporator pressures and outlet temperatures were used for the predictions of both cycles. However, note that since p_{out} does not have meaning in the

B | Complementary Analyses

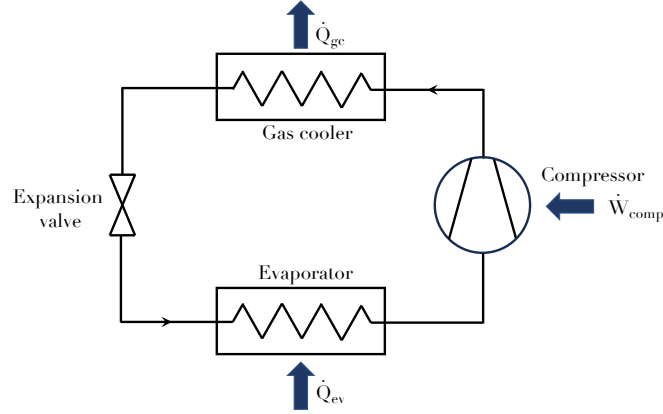


Fig. B.6 Schematic of the classical 4-components refrigeration cycle.

case of the four-components cycle, COP_{basic} is independent of it. It can be seen that under transcritical operation, the maximum COP improvement ratio (blue star) is found at lower gas cooler pressures than the maximum absolute COP point of the ejector cycle (black star), along the

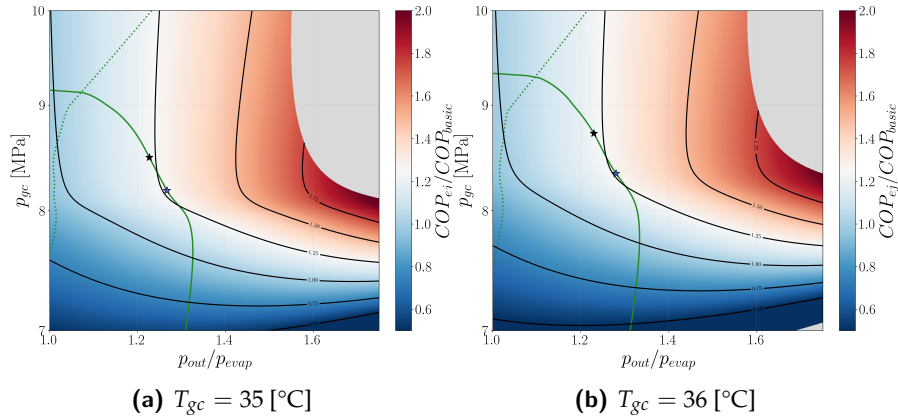


Fig. B.7 Maps of the COP improvement ratio of the ejector cycle compared to the classical cycle, as a function of p_{gc} or p_{cond} and the compression ratio p_{out}/p_{evap} . Operation curves are plotted in plain green line, and the on/off-design limit in dotted green line. Iso-COP ratios are plotted in plain black. The maximum COP and maximum COP improvement along the operation curve are highlighted by the black and blue stars, respectively.

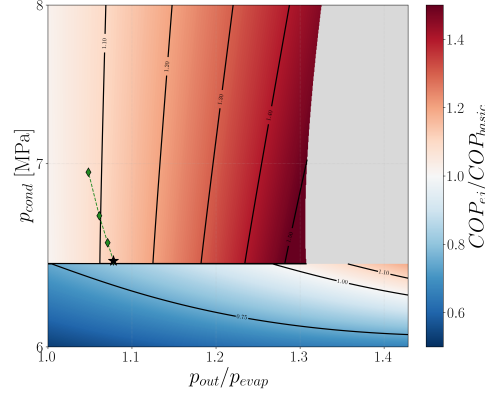


Fig. B.8 Maps of the COP improvement ratio of the ejector cycle compared to the classical cycle, as a function of the condenser pressure p_{cond} and the compression ratio p_{out}/p_{evap} . The operation curve is plotted in plain green (diamonds and dashed line). Iso-COP ratios are plotted in plain black. The maximum COP and maximum COP improvement along the operation curve (superimposed) are highlighted by the black star.

operation curve. There is however little difference in the improvement ratio values. For example, at $T_{gc} = 35$ [°C], the maximum absolute COP point of the ejector cycle is at $COP_{ej}/COP_{basic} = 1.240$ whereas the maximum ratio along the operation curve is at $COP_{ej}/COP_{basic} = 1.265$. As for the subcritical case, Figure B.8 indicates that the maximum COP improvement ratio along the operation curve occurs when the primary inlet is at saturated liquid conditions (refer to the explanations of Chapter 4), which coincides with the position of the maximum COP.



An Improved Thermodynamic Model for Supersonic Real-Gas Ejectors using the Compound-Choking Theory

The following article is largely based on research that was performed as a part of the Master's thesis of the candidate. The article has been written and published into the Energy journal during the Ph.D. thesis, and corresponds to reference [110].

3.1 Introduction

Much as they may offer a compelling alternative to traditional compression devices, ejectors are nonetheless characterized by complicated fluid dynamics, and some of the mechanisms at play within the ejector remain insufficiently understood, which hinders the performance of the global system [15]. Though the most straightforward approach to acquire data might be to perform experiments, such a strategy would not be economically advantageous as it would require too much time and material resources [30]. Instead, numerical methods seem to be the most profitable way to generate results. To this end, using thermodynamic models is the easiest and fastest way to give a first rough appreciation of ejector performance and/or to design them.

Ejectors are passive devices used to suck and compress fluids: a primary stream transfers a part of its energy and momentum to a secondary stream through viscous shearing and suction into the low pressure jet, leading to complex turbulent mixing phenomena in the mixing chamber [127]. During this process, the flow goes through a series of oblique shock waves that interact with the shear layer, thus re-compressing the fluid [24]. Because ejectors are used as entrainment devices, a convenient quantity to characterize their performance is their entrainment ratio $\omega = \dot{m}_s / \dot{m}_p$. To outline the different regimes of an ejector, it is convenient to draw its characteristic curves, which depict the evolution of the entrainment ratio as a function of the back-pressure. Figure C.1 depicts a typical ejector characteristic curve. Depending on the operating conditions and on the internal geometry of the ejector, the secondary flow might become choked as well [31]. As a result, below a certain value of the back-pressure, the secondary flow also becomes independent of the upstream conditions. This particular value of the back-pressure at which, given a particular stagnation pressure ratio $p_{p,0} / p_{s,0}$, the secondary flow becomes choked, is referred to as the *critical pressure* denoted by p_{out}^* . This phenomenon also implies that below p_{out}^* , the entrainment ratio becomes constant and the ejector is said to operate in the *on-design* regime or *critical mode*. Above the critical pressure, the ejector is influenced by the back-pressure. When the latter is increased, a shock wave moves into the mixing chamber, interacting with the mixing and boundary layers and hindering the secondary mass flow. The ejector is then said to operate in the *off-design* regime or *sub-critical mode*. If the back-pressure

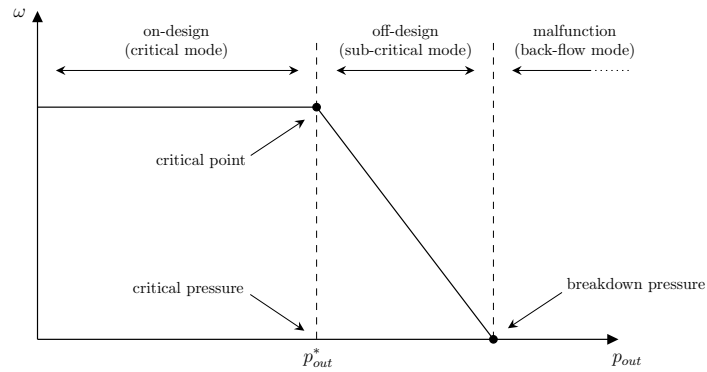


Fig. C.1 Typical characteristic curve of an ejector.

is increased above a threshold value referred to as the *breakdown pressure*, the primary flow reverses back into the suction chamber. This case corresponds to a malfunction of the ejector. The interested reader can refer to the recent reviews of Besagni et al. [17], Ameer et al. [3, 4] and Grazzini et al. [66] for more details about the applications, functioning and modeling of supersonic ejectors.

The first one-dimensional mathematical model of an ejector was introduced by Keenan et al. [77] in 1950. It was based on the application of mass, momentum and energy conservation equations, with the use of isentropic flow relations. This model has been used as a theoretical basis in ejector design since then. They compared constant-pressure mixing and constant-area mixing and deduced that the former performed better. However, the model of Keenan et al. [77] was unable to provide information on the choking phenomenon at play within a supersonic ejector [72].

Munday and Bagster [116] later proposed modifications to the model of Keenan et al. [77]. Their theory assumed that the two streams do not mix right away at the exit of the primary nozzle, but they rather conserve their integrity until a particular downstream section. It was postulated that an hypothetical throat is formed by the primary flow and the ejector wall, and that the secondary stream reaches a sonic velocity at that particular location (Fig. C.2). The two streams then mix at constant pressure. This phenomenology is somewhat related to the *choked secondary flow* pattern that was discovered experimentally by Fabri and Siestrunk [54] in 1958. Since the presence of an hypothetical throat constitutes the basis of numerous mathematical models, the choking mechanism associated with this regime is often referred to as *Fabri-choking* [84].

Based on those early works, a number of first generation thermodynamic models were proposed; Eames et al. [49] introduced in 1995 a model that included irreversibilities due to friction losses by using isentropic efficiencies; Huang et al. [74] developed a model of double-choking that also took irreversibilities into account, but for which they considered that the mixing phenomenon occurred inside the constant area duct; Rogdakis and Alexis [131] introduced a first real gas thermodynamic model with general conservation equations. However, those models could only predict the ejector performance at critical mode operation. In 2013, Chen et al. [29] introduced a model to predict the ejector performance at critical and sub-critical operational regimes. Their model was also based on the presence of an hypothetical throat inside the constant area duct. For the sub-critical operating regime, this hypothesis was conserved. The off-design performance

was obtained by using a mixing efficiency dependant on the back-pressure of the ejector. Perfect gas behavior was assumed and isentropic efficiencies were used to take friction losses into account. A few years later, Chen *et al.* [30] extended the model to real gas thermodynamic properties.

As pointed out by Lamberts *et al.* [85], the *Fabri-choking* is used as the foundation of most thermodynamic ejector models, including all of the aforementioned models [6, 30, 33, 49, 74, 116, 131, 135, 143]. However, the Fabri-choking has only been experimentally observed once, by Lamberts *et al.* [84] and characterized by signature shock-wave patterns called lambda-shocks. Indeed, according to the same authors, in many works where on-design ejectors are studied, no apparent sonic section in the core of the secondary stream is observed. In addition, significant discrepancies remain between experiments and model predictions, with on-design entrainment ratio deviations up to 16% in [30], and a reported average deviation of 7.8% in [149] as two examples. Hence, the Fabri-choking is not necessarily representative of the actual phenomena occurring inside of a doubly choked ejector. In their article, Lamberts *et al.* [85] described a new choking theory for perfect gas based on the early work of Bernstein *et al.* [14] about the so-called *compound-choking* theory. This theory proposed by Lamberts *et al.* [85] for perfect gas ejectors was then extended to real gas ejectors by Fang [55] and Metsue [108] for CFD and thermodynamic modeling purposes, respectively. Very recently, Croquer *et al.* [34] also validated the compound-choking for single-phase gas refrigerants using both approaches. In the latter study, the authors demonstrated, neglecting friction, that the mean error on the predicted entrainment ratio was reduced to about 5% when using the compound-choking criterion, compared to a mean error of more than 17% when using the Fabri-choking criterion.

In the present paper, the compound-choking theory developed by Fang [55] is used for the first time to build a *real gas* thermodynamic model for both on- and off-design operating regimes. First, the ejector model is presented, along with the solving algorithm (Section 3.2). The model of Chen *et al.* [30] is modified to integrate the compound-choking theory. Then, the new model is used to shed light on the relationship between the Fabri-choking and compound-choking criteria. It is then calibrated on experimental data for supersonic ejectors working with R134a and air, and the results are discussed in details in Section 3.3. Lastly, it is demonstrated that using the compound-choking criterion is actually equivalent to maximizing the total mass flow rate within the ejector working with a perfect gas (Section 3.4), which is the physical characteristic of a choked flow. The paper ends by

some conclusions and future views in Section 3.5.

3.2 Ejector model and solving algorithm

Over the numerous thermodynamic models published in the literature, the model of Chen et al. [30] is preferred as a basis for the present research, with some improvements. First, the primary flow is solved by maximizing the mass flow rate instead of imposing a Mach number M equal to unity at the throat, which constitute the primary definition of a choked flow. Most notably, the secondary flow is using the compound-choking theory, instead of the Fabri-choking theory commonly adopted by thermodynamic models.

3.2.1 Assumptions

The flow within an ejector is quite complex and thus often requires the use of assumptions in order to solve the flow swiftly, which is the essence of thermodynamic models. The main assumptions used in the present work are :

1. The flow is one dimensional, steady and adiabatic. The inlet (primary and secondary) and outlet velocities are supposed to be negligible.
2. Friction losses along the walls and within the shear layer between the primary and secondary streams are taken into account through isentropic efficiencies (Fig. C.2): η_p for the primary nozzle (sections $0 \rightarrow e$); $\eta_{p,y}$ for the friction losses undertaken by the primary flow within the mixing chamber (sections $e \rightarrow y$); η_s for the friction losses undertaken by the secondary flow within the mixing chamber (sections $0 \rightarrow y$) and η_d for the diffuser (sections $2 \rightarrow d$). The mixing losses between the primary and secondary streams are taken into account by means of a loss coefficient η_m (sections $y \rightarrow m$).
3. Real gas properties are retrieved from the tabulated database COOL-PROP available in the Python library.
4. Primary and secondary streams do not start mixing up until a particular section –that will be referred to as *mixing section*– located inside the constant area duct. At that location, both pressures are assumed to be equal. The location of the particular section at which the mixing phenomenon begins is the location of the hypothetical throat that is well described in the literature [72]. This section is *compound-choked* if the ejector is working under critical regime.

C | An improved ejector thermodynamic model

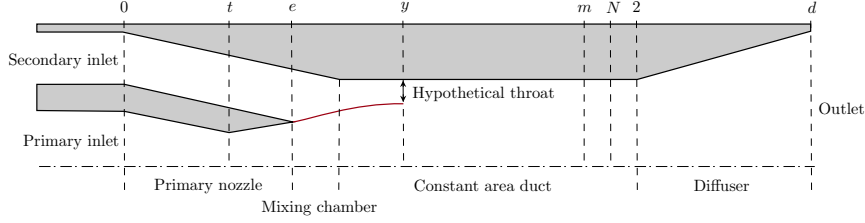


Fig. C.2 Schematic diagram of the ejector model (top half).

A schematic of the ejector, along with the notations that will be used in the following sections, is shown in Figure C.2. Since the primary flow is assumed to be choked, the primary mass flow rate $\dot{m}_p$ is constant and does not depend on any downstream quantity (i.e., it only depends on the primary stagnation conditions). The primary flow expands in the primary nozzle, and then further more in the mixing chamber until it reaches section y . The secondary flow is also –separately– expanded upon section y , and then only the mixing process starts. In other words, the two flows are essentially independent up until reaching section y . It is important to note that the position of the mixing section y is assumed to lie within the constant area section, whether or not the ejector is working in the on- or off-design regime. Then, the two flows start to mix at constant pressure, and are assumed to be completely mixed upon section m . If the flow is supersonic at section m , it consequently goes through a normal shock at section N , located in the constant area section as well. The flow thus reaches the diffuser inlet –section 2– at a subsonic speed. It then further expands in the diffuser, where the flow velocity is further decreased and the pressure recovered.

3.2.2 Modeling of on-design operation using the compound-choking criterion

Primary nozzle

The flow in the primary nozzle can be solved from the stagnation conditions and the isentropic efficiency governing the flow in this part. It is convenient to set the stagnation conditions with the primary pressure $p_{p,0}$ and the primary temperature $T_{p,0}$. When working with saturated fluids, it is sometimes more relevant to define stagnation conditions with the quality of the fluid $q_{p,0}$. For the sake of simplicity, the stagnation conditions will be defined with $p_{p,0}$ and $T_{p,0}$ in the following.

First, the enthalpy and entropy of the primary flow at the inlet can be

computed from the pressure and temperature:

$$h_{p,0} = h(p_{p,0}, T_{p,0}), \quad (C.1)$$

$$s_{p,0} = s(p_{p,0}, T_{p,0}). \quad (C.2)$$

For a given pressure p_p and assuming an isentropic expansion, the enthalpy at said pressure can be computed:

$$h_{p,is} = h(p_p, s_{p,0}). \quad (C.3)$$

Knowing the isentropic efficiency of the primary nozzle η_p , one can then compute the enthalpy resulting from the non-isentropic expansion process:

$$h_p = h_{p,0} - \eta_p (h_{p,0} - h_{p,is}). \quad (C.4)$$

The density along the expansion can then be computed from the pressure and enthalpy. From the conservation of total enthalpy, one can also compute the flow velocity:

$$\rho_p = \rho(p_p, h_p), \quad (C.5)$$

$$V_p = \sqrt{2 (h_{p,0} - h_p)}. \quad (C.6)$$

In order to solve the flow, the hypothesis of choked primary flow has then to be used. The classical way to impose such a condition is to set the Mach number to unity at the nozzle throat. Although this is the approach taken in the model of Chen *et al.* [30], one prefers to impose the choking condition by the maximization of the mass flux. This approach presents two advantages. First, one does not require to know the speed of sound at the throat for the computation of the primary mass flow rate, which can sometimes be problematic for two-phase flows, as the COOLPROP library is flawed for thermodynamic conditions close to the saturation curve. Then, if one considers a non-isentropic expansion, the sonic section is not actually located at the geometric throat of the nozzle, but rather at a certain distance downstream. Imposing a Mach number equal to unity at the throat would consequently lead to an error in the computation of the primary mass flow rate. By rather directly maximizing the mass flow rate, this problem is avoided and the physical definition of a choked flow is preserved. Indeed, in the case of an isentropic nozzle flow, it can be shown that maximizing the mass flow rate per unit area is equivalent to imposing $M = 1$ at the throat.

C | An improved ejector thermodynamic model

The mass flux (i.e., the mass flow rate per unit area) is defined as :

$$G = \rho V. \quad (\text{C.7})$$

From Eqs. (C.1) through (C.7), the expansion of the fluid in the primary nozzle can be computed. Figure C.3 shows the typical behavior of G along an expansion with R134a as the working fluid for various stagnation conditions. One can observe that the mass flow rate per unit area has a maximum along the expansion. Furthermore, this maximum gets higher and closer to the stagnation pressure as the stagnation temperature gets lower, i.e. the stagnation conditions get to the left hand side of the saturation curve. Indeed, as the temperature gets lower, the fluid transitions from a superheated vapour (for $T_{p,0} = 100\text{ }^{\circ}\text{C}$) to a denser subcooled liquid (for $T_{p,0} = 65\text{ }^{\circ}\text{C}$ and $T_{p,0} = 60\text{ }^{\circ}\text{C}$). The much higher density of a liquid explains why the maximum of G gets higher. In addition, one can see that as $T_{p,0}$ gets lower, the maximum of G shifts to the left (i.e., at a pressure closer to the stagnation pressure).

For stagnation conditions where the fluid is highly subcooled, there is actually somewhat of an angular point at the location of the maximum, as

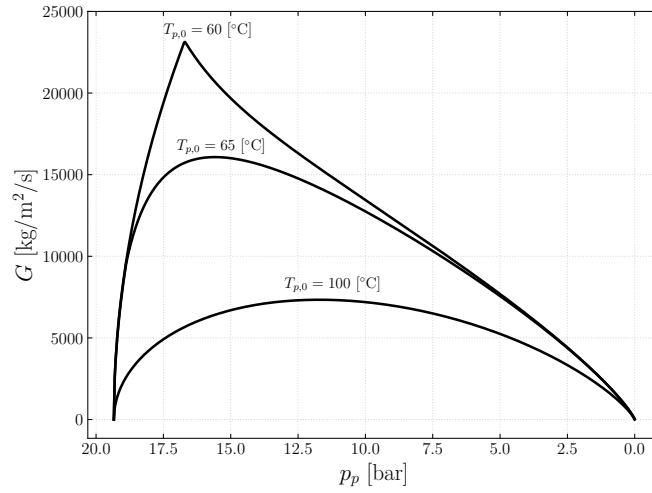


Fig. C.3 Variations of the mass flux G as a function of the primary flow pressure p_p for three stagnation temperatures. Results obtained for R134a with $p_{p,0} = 1.934\text{ [MPa]}$ and $\eta_p = 0.97$.

the fluid flashes along the expansion. By doing so, the fluid loses a great deal of density in an almost discontinuous fashion. This brings forward the need to compute very accurately the position of the maximum, because due to this angular point, a slight imprecision will lead to a substantial error in the mass flow rate. To compute efficiently the maximum mass flux, it is convenient to use the fact that G has only one maximum. Therefore, one can proceed iteratively by computing $G = f(p_p)$ for a reduced amount of linearly spaced pressures p_p , and then narrowing the interval on p_p where the maximum is located until finding the solution with the desired precision.

Knowing the maximum mass flow rate per unit area $G_{p,max}$ and the throat area of the nozzle A_t , the mass flow rate for the choked primary nozzle is found by:

$$\dot{m}_p = G_{p,max} A_{p,t}. \quad (C.8)$$

The throat thermodynamic state is then fully solved, as $G_{p,max}$ provides the knowledge of the throat pressure $p_{p,t}$, which can later be used to find the throat enthalpy $h_{p,t}$ by the use of Eqs. (C.3) and (C.4). The velocity at the throat is then found using Eq. (C.6).

It is important to note that the COOLPROP library is faulty near the critical point, meaning that requesting the computation of a thermodynamic quantity near said region generates an error. In order to circumvent this issue and prevent the whole operation to stop, it was chosen to manage this error by assuming that the thermodynamic quantities near the vicinity of the faulty region are equal to the quantities slightly above or slightly below the critical point. Except in the rare case where the maximum of G is located exactly at the critical point, this procedure does not lead to any loss of accuracy.

The nozzle exit conditions are found by further expanding the flow from the known state at the throat. Knowing the exit section area $A_{p,e}$, the exit state of the fluid is found by using the mass and total enthalpy conservation equations. Indeed, the flow must satisfy :

$$V_{p,e} = \frac{\dot{m}_p}{\rho_p A_{p,e}}, \quad (C.9)$$

and

$$V_{p,e} = \sqrt{2(h_{p,t} - h_p) + V_{p,t}^2}, \quad (C.10)$$

where h_p and ρ_p can be computed along the expansion (i.e., as a function

C | An improved ejector thermodynamic model

of p_p) in the divergent of the nozzle with the use of Eqs. (C.4) and (C.5), respectively. The solution $V_{p,e}$ is found by selecting the unique value that allows Eqs. (C.9) and (C.10) to be satisfied simultaneously. Once again, the state at the primary nozzle exit is then fully defined, as the value of $V_{p,e}$ provides direct knowledge of $\rho_{p,e}$ and $h_{p,e}$.

Mixing chamber

The on-design conditions at section y (i.e., the mixing section) can be found using the compound-choking criterion for real gas derived in [34], i.e.:

$$\beta = p_y \left(\frac{A_{p,y}}{(\rho_{p,y} V_{p,y}^2)} (1 - M_{p,y}^2) + \frac{A_{s,y}}{(\rho_{s,y} V_{s,y}^2)} (1 - M_{s,y}^2) \right) = 0, \quad (\text{C.11})$$

where the secondary flow properties at section y are computed from the secondary inlet conditions and using the prescribed value of p_y (please refer to Croquer et al. [34] for more details). Once the value of p_y is found with sufficient precision (i.e., $\beta \leq \epsilon$, with ϵ the error tolerance), all properties at section y are known, and the secondary mass flow rate can be computed by:

$$\dot{m}_s = \rho_{s,y} V_{s,y} A_{s,y}, \quad (\text{C.12})$$

which allows to determine the on-design entrainment ratio $\omega = \dot{m}_s / \dot{m}_p$. Figure C.4 shows the flowchart of the algorithm described here. Note that the procedure to compute the critical back pressure will be presented in the next section (i.e., the modeling of the sub-critical regime), as it is the same for on- and off-design operations.

3.2.3 Modeling of off-design operation

Similarly to the previous subsection, the present model is based on the one published by Chen et al. [30]. However, their original model suffers from mass conservation issues between sections y and m . Indeed, because said model assumes that the mixing process between primary and secondary flows occurs at a constant pressure, the associated equation (i.e., $p_y = p_m$) is added to the system to solve the flow at section m . However, by doing so, the mass conservation equation is omitted; momentum, energy and pressure constraints are enough to solve the system, resulting in the fact that $\dot{m}_p + \dot{m}_s \neq \rho_m V_m A_y$. To overcome this issue, the present model does not consider that the mixing process occurs at constant pressure. Instead,

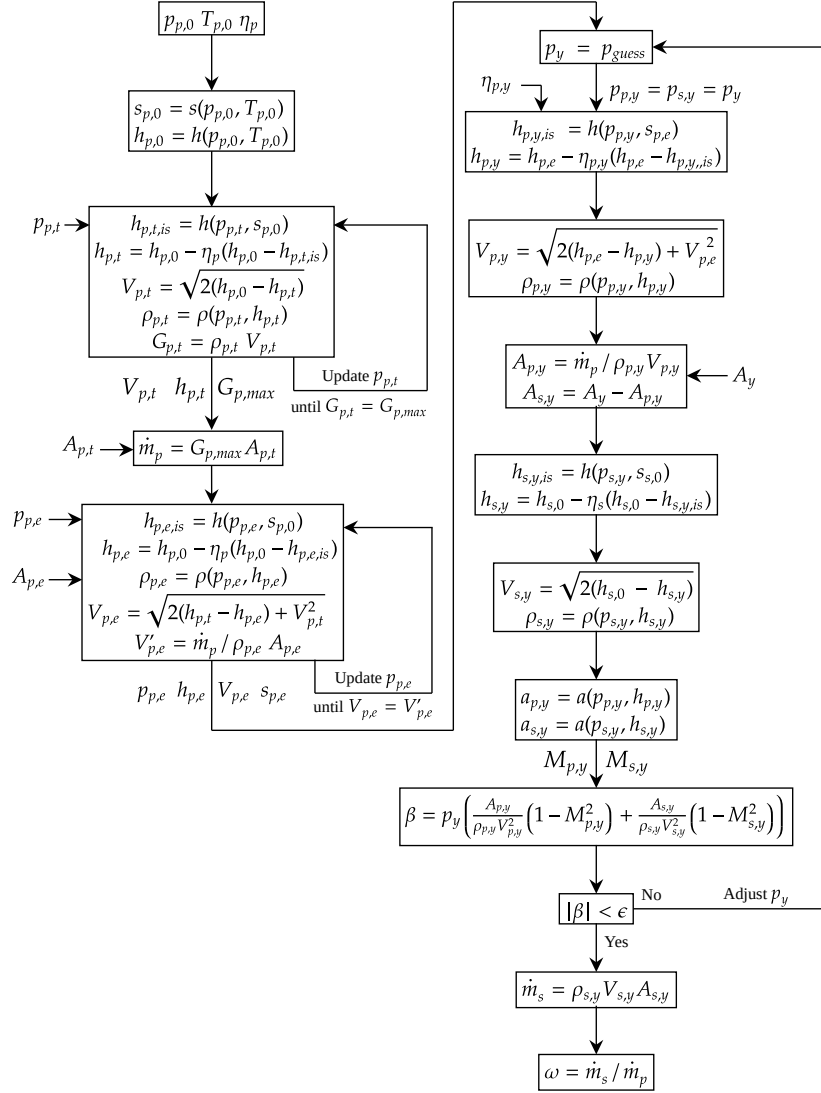


Fig. C.4 Flowchart of the model for on-design operations using the compound-choking criterion (Fig. C.2).

the mass conservation equation is re-introduced to solve the flow between sections y and m .

C | An improved ejector thermodynamic model

Unlike in on-design operation, the off-design ejector performance depends on downstream conditions (i.e., the back pressure p_{out}). Indeed, if the ejector is operating in the off-design regime, information will travel from the end of the diffuser up to the mixing section. The mixing pressure p_y will consequently be higher when the ejector is operating in off-design regime than when it is operating in on-design regime, and the secondary mass flow rate will thereby be impacted. The entrainment ratio will thus be dependant on the back pressure. As mentioned previously for on-design operation, it is not required to solve the flow downstream of section y in order to compute the entrainment ratio. This is not true if one wishes to obtain ω for a particular back pressure. In order to determine the ejector regime and, if necessary, compute the entrainment ratio for off-design operation, the flow has to be solved up to the diffuser exit, i.e. section d (Fig. C.2). As a reminder, the condition for the ejector to be in on-design regime is given by:

$$p_{out} < p_{out}^*, \quad (C.13)$$

where p_{out}^* is the critical back pressure. Hence, the critical back pressure has to be computed to assess the operating regime. First, the thermodynamic states and velocities of the primary and secondary flows are computed using the on-design model, that is, using the compound-choking theory. Then, properties are computed at section m , that is the particular section located inside the constant area duct at which primary and secondary flows are assumed to be completely mixed. State m therefore constitutes one single state, without any distinction between the two flows.

As stated above, the assumption of constant mixing pressure in the original paper of Chen *et al.* [30] is lifted and replaced by the mass conservation equation. This implies that an additional term has to be added to the momentum conservation equation, to take into account the pressure difference between sections m and y . This involves that state m has to be solved using an iterative method, as V_m depends on the unknown pressure p_m . State m is therefore defined by four equations. First, the conservation of mass writes:

$$\rho_m V_m A_y = \dot{m}_p + \dot{m}_s. \quad (C.14)$$

Then, the momentum conservation equation writes:

$$V_m = \eta_m \frac{\dot{m}_p V_{p,y} + \dot{m}_s V_{s,y} + (p_y - p_m) A_y}{\dot{m}_p + \dot{m}_s}. \quad (C.15)$$

Note at this point that η_m does not need to be a linear function of p_{out} as it was the case for the model of Chen *et al.* [30]. Instead η_m is assumed to be constant. The third equation is the total enthalpy conservation equation:

$$h_m = \frac{\dot{m}_p h_{p,0} + \dot{m}_s h_{s,0}}{\dot{m}_p + \dot{m}_s} - \frac{V_m^2}{2}, \quad (C.16)$$

and the last equation is the equation of state linking ρ_m , p_m and h_m :

$$\rho_m = \rho(p_m, h_m). \quad (C.17)$$

To solve this system of equations, the pressure p_m is guessed. The flow velocity V_m is then computed from Eq. (C.15), along with the enthalpy h_m using Eq. (C.16). The flow density ρ_m can then be obtained from Eq. (C.17). The pressure p_m is modified until Eq. (C.14) is satisfied. Practically, the solution is found by restraining at each iteration the solution interval on p_m until finding the minimum (or here, also the zero) of $|\rho_m V_m A_y - (\dot{m}_p + \dot{m}_s)|$.

After the mixing, the flow may be or not supersonic. However, it has to be subsonic when entering the diffuser, otherwise it would actually act as a divergent nozzle, thereby accelerating the flow. However, the goal is to recover the pressure at the ejector exit. For the 0-D model, if the flow is supersonic at section m , it was chosen to re-compress it through a single normal shock located at the end of the constant area duct (section N). Note that sections m , N and 2 are virtually at the same location, but were drawn separately in Figure C.2 for the sake of readability.

Because the flow may already be subsonic upon section m , it was chosen to check the Mach number at said section and compute the normal shock only if $M_m > 1$. Indeed, if the flow at section m is subsonic, it is unnecessary to solve the equations for a normal shock. In that case, the subsonic flow at the diffuser inlet (section 2) is indistinguishable from the flow at section m . On the other hand, if the flow is indeed supersonic at section m , the mass, momentum and total enthalpy conservation equations have to be solved to compute the flow at section 2. This has to be performed using an iterative scheme. First, the fluid density is guessed at section 2:

$$\rho_2 = \rho_{guess}, \quad (C.18)$$

with ρ_{guess} chosen higher than ρ_m . The flow speed is then computed from

C | An improved ejector thermodynamic model

the conservation of mass:

$$V_2 = \frac{\rho_m V_m}{\rho_2}, \quad (\text{C.19})$$

From the conservation of total enthalpy, the enthalpy is computed as:

$$h_2 = h_m + \frac{V_m^2}{2} - \frac{V_2^2}{2}, \quad (\text{C.20})$$

and the pressure at section 2 is obtained from tabulated data by:

$$p_2 = p(\rho_2, h_2), \quad (\text{C.21})$$

The momentum conservation equation is then used to update the value of ρ_2 that was initially guessed:

$$\rho_2 = \frac{(\rho_m V_m^2 + p_m - p_2)}{V_2^2}. \quad (\text{C.22})$$

The latter value of ρ_2 is then re-injected in Eq. (C.19) and re-computed until convergence. State 2 being fully defined, the last step is to solve the flow within the diffuser. To this end, one must first retrieve the entropy at section 2 from tabulated data:

$$s_2 = s(p_2, h_2). \quad (\text{C.23})$$

The enthalpy at the diffuser exit (section d) for an isentropic compression denoted $h_{d,is}$ may be expressed using the classical definition of the isentropic efficiency η_d :

$$\eta_d = \frac{h_{d,is} - h_2}{h_d - h_2}. \quad (\text{C.24})$$

Then, applying the total enthalpy conservation equation:

$$h_d = h_2 + \frac{V_2^2}{2}, \quad (\text{C.25})$$

one finally gets:

$$h_{d,is} = h_2 + \eta_d \frac{V_2^2}{2}, \quad (\text{C.26})$$

where the assumption of negligible flow velocity at section d was used. The

pressure at the diffuser exit can finally be computed by:

$$p_d = p(h_{d,is}, s_2), \quad (C.27)$$

as the end pressure for the isentropic expansion is the same as that of the non-isentropic one. If the ejector is double-choked, the computed pressure

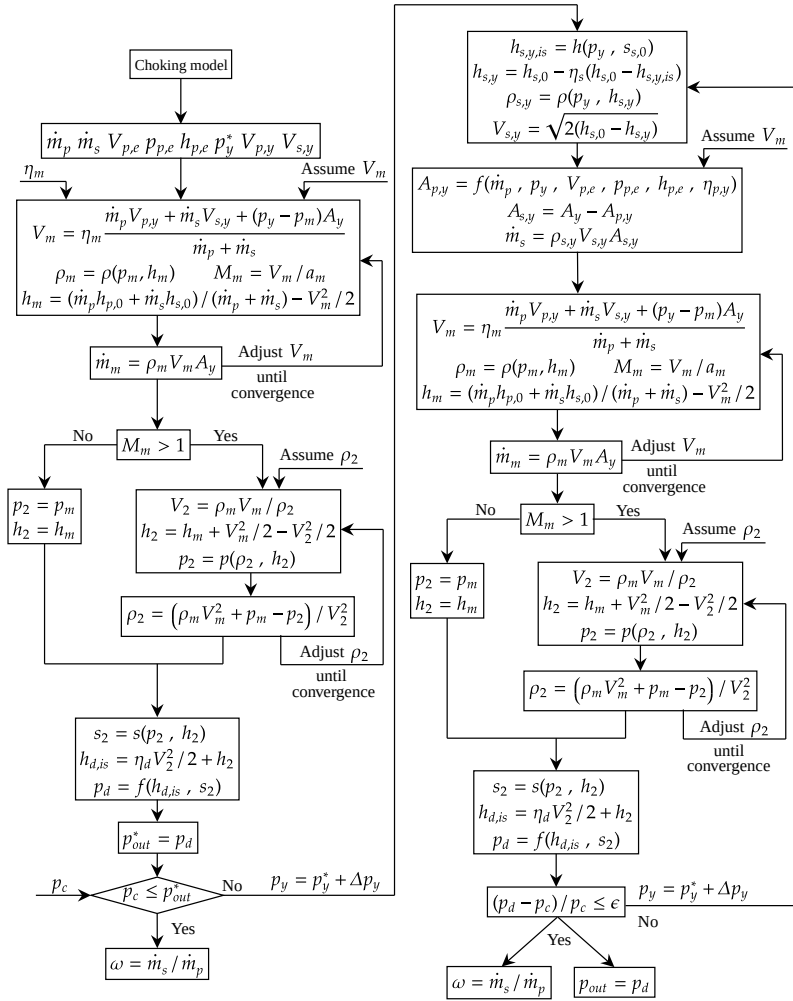


Fig. C.5 Flowchart of the model for off-design operation.

C | An improved ejector thermodynamic model

p_d actually corresponds to the critical back pressure p_{out}^* , and if the ejector is under sub-critical regime, one has that $p_d = p_{out}$.

For a given back pressure p_c , one can now determine if the ejector works in the on- or off-design regime. For the latter case, the pressure at the end of the diffuser must match the back pressure, which requires to solve the flow in an iterative way until finding the pressure p_y that satisfies :

$$\frac{|p_d - p_c|}{p_c} \leq \epsilon, \quad (C.28)$$

with ϵ the error tolerance. As mentioned previously, the mixing pressure p_y gets higher as the back pressure gets higher when the ejector is working in the off-design regime. Pressure p_y is therefore updated at each iteration until satisfying Eq. (C.28). Figure C.5 summarizes the computation algorithm of the new off-design model.

3.3 Validation of the thermodynamic model for single-phase ejectors

3.3.1 Relation between Fabri-choking and compound-choking

It is now proposed to explain in more details the link between Fabri-choking and compound-choking. To do that, the air ejector geometry of the test bench at Université catholique de Louvain and considered by Lamberts *et al.* [84, 85] is modeled for $p_{p,0}/p_{s,0} = 4.5$ and with $\eta_m = 0.92$. All other efficiencies are set to 1. First, one can plot the evolution of the mixing pressure as a function of the back pressure as displayed in Figure C.6a. One can notice that the design mixing pressure p_y^* , and therefore the on-design plateau, are higher when using the compound-choking criterion. This can be interpreted as follows: as thoroughly discussed in [34], the compound-choking predicts the choking of the ejector for secondary Mach numbers lower than 1 at the aerodynamic throat (section y). Hence, the pressure at said location must be higher than that in the case of the Fabri-choking (i.e., $M_{s,y} = 1$) because the secondary flow has been less expanded. In addition, note that as the back pressure tends to the breakdown pressure, the mixing pressure tends to reach the secondary stagnation pressure. As expected, when $p_y = p_{s,0}$, there is no pressure gradient to expand the secondary flow, hence $\dot{m}_s = 0$ and the entrainment ratio gets to zero.

Then, Figure C.6b presents the evolution of the entrainment ratio as a

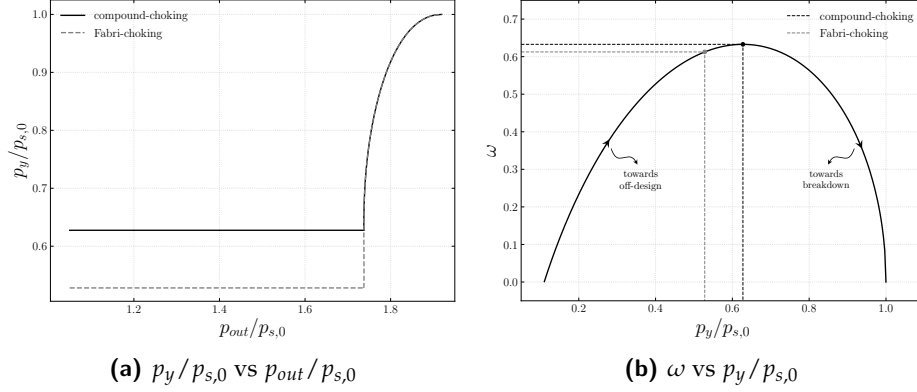


Fig. C.6 Comparison between Fabri-choking and compound-choking for $p_{p,0}/p_{s,0} = 4.5$. The working fluid is air and $\eta_m = 0.92$. The positions of the critical conditions have been highlighted on the ω -curve.

function of the mixing pressure. As a reminder, ω can be computed as a function of the mixing pressure and the stagnation conditions only. Then, the positions of the critical conditions can be located for both choking criteria. Those are represented by dots on the curve. One can now clearly see why the compound-choking criterion systematically predicts higher entrainment ratios than the Fabri-choking criterion. Indeed, the entrainment ratio predicted by the compound-choking is located exactly at the maximum of the curve. This means that, if the transformations are isentropic until the mixing section, satisfying the compound-choking criterion will lead to the maximization of the total mass flow rate within the ejector. Indeed, since the primary flow is choked, maximizing ω is equivalent to maximizing $\dot{m}_s$ and therefore $\dot{m}_p + \dot{m}_s$.

On the other hand, the Fabri-choking mixing pressure at the critical condition p_y^* is slightly lower than that of the maximum. Although not discussed in the article of Chen et al. [30], it was found, by re-implementing their model, that because the Fabri-choking criterion does not maximize the entrainment ratio (and thus the total mass flow rate), the near-critical off-design part of the characteristic curve contains a spurious overshoot. Indeed, as one gets further into the off-design part of the characteristic curves, the mixing pressure p_y gets higher. Hence, starting from the Fabri-choking critical point (Fig. C.6b) and following the curve towards the right, one eventually reaches the maximum (i.e., the compound-choking critical point).

By the same token, it is the authors understanding that other thermodynamic models based on the Fabri-choking criterion and modeling off-design operation should logically present similar overshoots, unless they have been manually cropped. This spurious overshoot will be observed and further discussed in the following.

3.3.2 Influence of the isentropic efficiencies on the characteristic curves

In order to efficiently calibrate the model, it is relevant to assess the individual effect of each efficiency on the shape of the characteristic curves by varying one of the efficiencies at a time. Figure C.7 displays the influence of the four isentropic efficiencies (i.e., η_p , η_s , $\eta_{p,y}$ and η_d) and the mixing efficiency η_m . The curves for the counterpart Fabri-choking model (i.e., imposing $M_{s,y} = 1$) have also been displayed for comparison purposes. Note that, if not mentioned, the isentropic efficiencies are set to 1 by default and η_m to 0.95.

One can then observe the influence of the different isentropic efficiencies and the results may be summarized as follows:

- When decreasing η_p , the primary mass flow rate is decreased, as the flow velocity at the primary throat gets lower. The on-design entrainment ratio therefore increases. The effect of friction in the primary nozzle is somewhat equivalent to having a lower primary stagnation pressure. This explains the fact that the critical back pressure gets lower.
- When decreasing η_s , the on-design entrainment ratio gets lower, as the secondary mass flow rate is decreased. The back pressure is closely related to the total mass flux going through the ejector. Thus, a lower secondary mass flow rate also results in a decrease of the critical back pressure. Note also that the off-design curves all have the same breakdown pressure. This is explained by the fact that at the breakdown pressure, $\dot{m}_s = 0$ and the secondary flow does not influence the total flow anymore. This is not true when η_p varies, which is why the breakdown pressures in Figure C.7a are not the same. Moreover, one can observe that the spurious overshoot that was previously discussed in the case of the Fabri-choking curves is also present in the compound-choking curves. This is actually due to the fact that, as explained in Croquer et al. [34], the compound-choking criterion as expressed in Eq. (C.11) is not rigorously correct if one considers non-isentropic flows. Indeed, because the criterion in Eq. (C.11) was obtained with

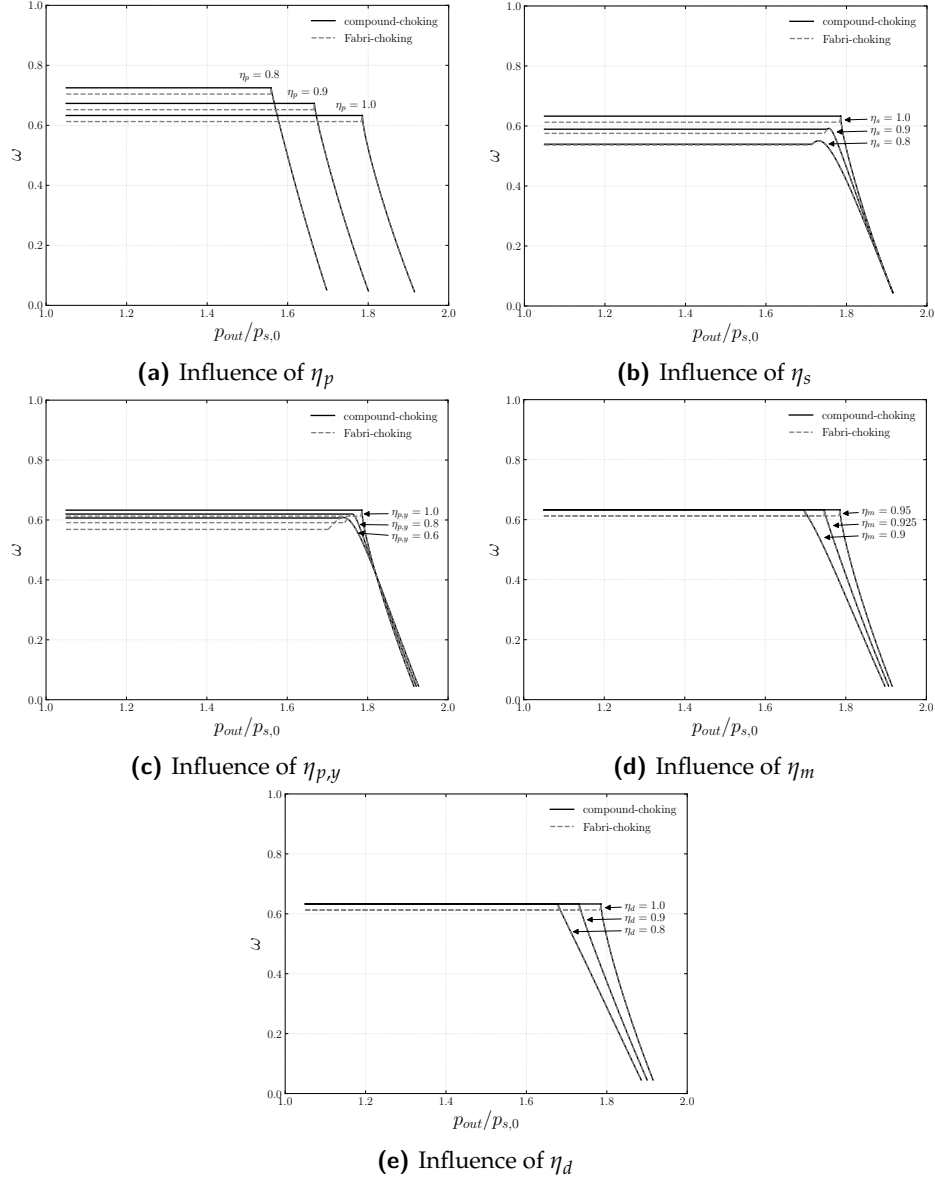


Fig. C.7 Influence of the different isentropic efficiencies on the characteristic curves using the compound-choking based model. The Fabri-choking model is also displayed for comparison purpose.

C | An improved ejector thermodynamic model

the hypothesis of isentropic flow, when friction losses are introduced into the model by means of the isentropic efficiencies, Eq. (C.11) is no longer rigorously accurate, in the sense that the compound-choking indicator β is no longer calculated in compliance with its definition, given in [14]. If Eq. (C.11) is nonetheless utilized with non-unity η_s or $\eta_{p,y}$, as it is the case for the curves in Figs. C.7b and C.7c, the spurious overshoot will be present on the compound-choking curves as well because Eq. (C.11) will not predict the maximum secondary mass flow rate. However, it will actually be demonstrated in the next section that using a *corrected* expression of β does maximize the secondary mass flow rate. Therefore, when dealing with non-isentropic expansions, the correct choking criterion should be that the total mass flow rate is maximized, which is in concordance with Eq. (C.11), with the proper computation of β .

- Decreasing $\eta_{p,y}$ has a somewhat similar effect to decreasing η_s , but to a lesser extent. However, none of the two mass fluxes are directly hindered by this efficiency. An intuitive way to explain this is that, as $\eta_{p,y}$ gets lower, the primary flow is expanded less efficiently in the mixing chamber. Thus, friction hinders the primary flow expansion (the flow velocity is lower), so that the primary flow mixing area $A_{p,y}$ must get higher to maintain the mass flow rate. Conversely, the secondary flow mixing area $A_{s,y}$ gets lower, therefore decreasing the secondary mass flow rate and hence the entrainment ratio.
- Lowering η_m does not influence the on-design entrainment ratio, as the latter does not depend on the mixing. As η_m decreases, the critical back pressure decreases. Indeed, the friction interactions cause a loss of stagnation pressure, thereby lowering the back pressure. This is comparable to a Fanno flow.
- The effect of η_d is quite similar to that of η_m . Lowering η_d tends to decrease the critical back pressure.

At this stage, one chooses not to use the diffuser isentropic efficiency η_d for later calibration. Indeed, this efficiency has the same influence on the characteristic curves as η_m . Furthermore, in real ejectors, the diffuser is usually well designed, meaning that it can reasonably be assumed that the flow is isentropic.

3.3.3 Fitting to R134a ejector experimental data

To calibrate the characteristic curves for ejectors working with R134a, the experimental data of Garcia del Valle *et al.* [60] are used as reference. Three different geometries were presented in the original article. However, they differ only in shape; the areas at the sections of interest (Fig. C.2) are equal. For this reason, only one ejector can be modeled using the present 0-D model. The relevant ejector dimensions are thus $D_t = 2.0$ [mm], $D_e = 3.0$ [mm] and $D_y = 4.8$ [mm]. The stagnation conditions for the experiments are $(T_{sat})_{p,0} = 84.38$ °C and $(T_{sat})_{s,0} = 10$ °C with a superheating of 10 °C. Superheating the vapour ensures that the flow does not condense within the ejector.

It was found that an accurate calibration could be performed by using only three parameters, that are, $\eta_p = 0.977$, $\eta_s = 0.89$ and $\eta_m = 0.813$. The value of $\eta_{p,y}$ is thus maintained to 1. Note that these values appear to be plausible for real ejectors. Indeed, the primary nozzle flow is almost isentropic and the secondary flow slightly less due to the more complex geometry. The most limiting factor remains the mixing efficiency.

Figure C.8 shows the results of the calibration, along with the CFD results

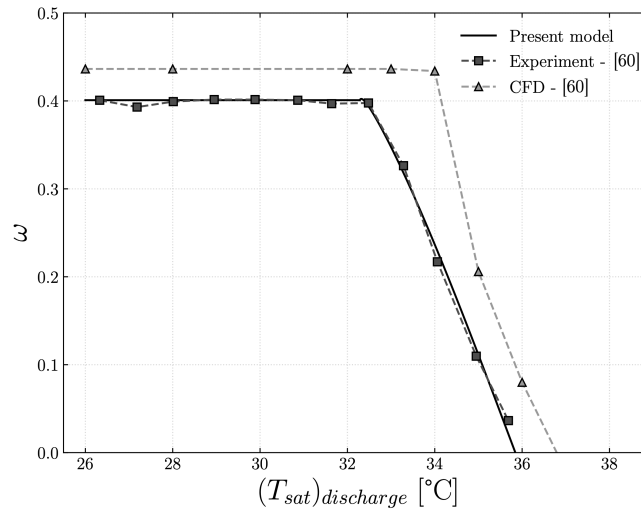


Fig. C.8 Characteristic curve obtained for an ejector working with R134 with $(T_{sat})_{p,0} = 84.38$ °C, $(T_{sat})_{s,0} = 10$ °C, $\eta_p = 0.977$, $\eta_s = 0.89$ and $\eta_m = 0.813$. Comparison between the present numerical model, the CFD of Croquer *et al.* [34] and the experimental data of Garcia del Valle *et al.* [60].

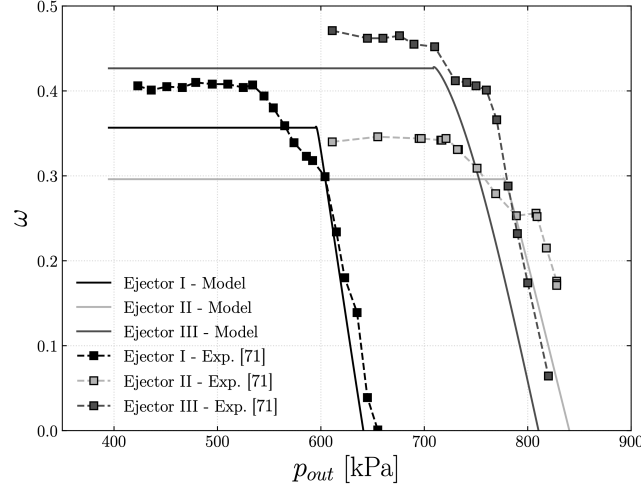


Fig. C.9 Characteristic curves obtained for three ejectors working with R134 with $\eta_p = 0.977$, $\eta_s = 0.89$ and $\eta_m = 0.813$. Comparison between the present thermodynamic model and the experimental data of Hakkaki-Fard et al. [71].

obtained by Croquer et al. [34]. The model fits quite well the experimental data of Garcia del Valle et al. [60], even better than the CFD results that tend to overestimate the entrainment ratio.

It is now proposed to plot the characteristic curves for the ejectors of Hakkaki-Fard et al. [71] using the calibration parameters found for the ejector of Garcia del Valle et al. [60], with the aim of determining if the calibration stays accurate. The three ejector geometries and operating conditions that were tested experimentally are summarized in Table C.1. Figure C.9 shows the results for the three ejectors. One can observe that, although the model does not predict the entrainment ratio as accurately as for the ejector of Garcia del Valle et al. [60], it nevertheless gives a good approximation. The model appears to underestimate the on-design entrainment ratio, but the off-design part of the characteristic curves seems to fit quite nicely. More precisely, the slopes of the off-design curves are quite accurate, and the model even overlaps the experiments for Ejector I. One could argue that the calibration process should yield better results if it were performed on one of the ejectors of Hakkaki-Fard et al. [71]. However, by doing so, the predictions of the characteristic curves for the two other ejectors were found to be quite poor, adding to the fact that the experimental curves of Hakkaki-

	Ejector I	Ejector II	Ejector III
Primary pressure $p_{p,0}$ [kPa]	2900	2633	1934
Primary temperature $T_{p,0}$ [°C]	106	100	86
Secondary pressure $p_{s,0}$ [kPa]	265	350	415
Secondary temperature $T_{s,0}$ [°C]	50	25	30
Primary throat diameter D_t [mm]	5.63	7.09	8.03
Primary nozzle exit diameter D_e [mm]	7.85	9.70	11.35
Mixing section diameter D_y [mm]	16.4	16.4	16.4

Table C.1 Geometry and operating conditions for the three experiments of Hakkaki-Fard et al. [71].

Fard et al. [71] contain some rather unconventional double plateaus. Using the parameters obtained for the ejector of Garcia del Valle et al. [60] yields overall satisfactory predictions for the three ejectors of Hakkaki-Fard et al. [71].

3.3.4 Fitting to air ejector experimental data

The model was also calibrated on new experimental data obtained using the air ejector test bench at Université catholique de Louvain. As a reminder, the geometry of said ejector is given in the articles of Lamberts et al. [84, 85]. Again, the calibration could be performed by means of only three parameters, that are, $\eta_p = 0.977$, $\eta_s = 0.75$ and $\eta_m = 0.95$. As before, $\eta_{p,y}$ is set to 1. The relatively low value of η_s is likely to be caused by the peculiar geometry of the air ejector, adding to the fact that the secondary flow has to go through an angle of 90 degrees before entering the mixing chamber (see Lamberts et al. [84] for more details about the ejector setup). On the other hand, the quite high mixing efficiency may reflect that the mixing process is relatively efficient. It should however be reminded that η_m is not an isentropic efficiency, therefore the mixing process will generate entropy even if said efficiency is set to unity.

Figure C.10 shows the fitting results obtained by calibrating the parameters on the new experimental data gathered for $p_{p,0}/p_{s,0} = 3.5$. Note that the secondary stagnation conditions correspond to the atmospheric ones for this particular ejector, so that $p_{s,0} = 1$ [bar]. In addition, the curves for $p_{p,0}/p_{s,0} = 2.5$ and $p_{p,0}/p_{s,0} = 4.5$, for which the values of the efficiencies have been kept equal to those previously mentioned, have also been displayed. One can see that the calibration allows the model to fit relatively well the experimental curves for the three cases. The off-design slopes do

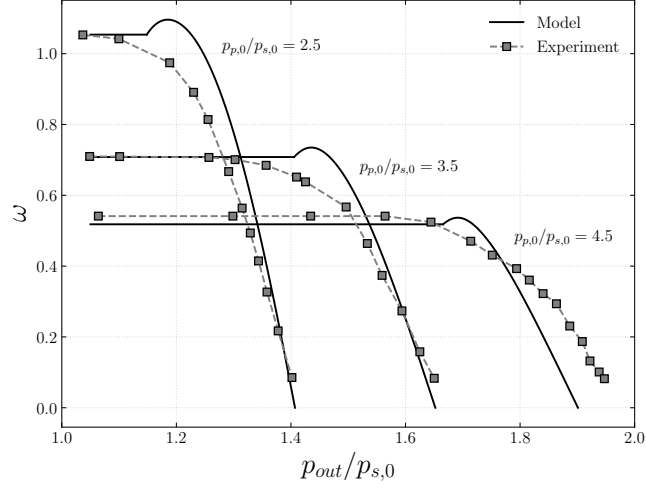


Fig. C.10 Characteristic curves obtained for the air ejector test bench of Université catholique de Louvain with $\eta_p = 0.977$, $\eta_s = 0.75$ and $\eta_m = 0.95$. Comparison between the present thermodynamic model and new experimental data.

however not match the experimental data as well as for the case of Garcia del Valle *et al.* [60] seen previously. The error remains however limited, and the general shape of the curves is relatively close to that of the experimental ones. The main issue with those curves is that there is a significant spurious overshoot near the critical point.

3.4 Relation between the compound-choking criterion and the maximization of the mass flow rate

In this section, it is proposed to perform an analytical study on the compound-choking criterion in the frame of non-isentropic perfect gas flows. The aim is to demonstrate the connection between the compound-choking criterion and the maximization of the mass flow rate within an ejector, which could be put in parallel with the definition of choking in the classical sense, i.e. for a simple nozzle.

3.4.1 Non-isentropic nozzle flow of a perfect gas

Before going towards ejectors and multi-stream flows, one first needs to develop the equations for non-isentropic nozzle flows for perfect gases. The

Relation between the compound-choking criterion and the maximization of the mass flow rate | 3.4

objective is to be able to determine the links between the differentials of all the physical quantities for such flows and the corresponding compound-choking criterion. In order to obtain an analytical solution for this problem, one will consider a polytropic efficiency, noted η_{pol} defined as:

$$\eta_{pol} = \frac{dh}{dh_{is}},$$

since one only deals with expansions. In the previous sections, isentropic efficiencies were used because these are more suited for global transformations. However, these two types of efficiencies (isentropic and polytropic) can be linked for an expansion of a perfect gas from pressure p_1 to p_2 through:

$$\eta = \frac{(p_2/p_1)^{\frac{(\gamma-1)\eta_{pol}}{\gamma}} - 1}{(p_2/p_1)^{\frac{\gamma-1}{\gamma}} - 1}. \quad (C.29)$$

The conservation equations in a control volume can be written as:

$$\frac{d\rho}{\rho} + \frac{dV}{V} + \frac{dA}{A} = 0, \quad (C.30)$$

$$\rho V dV + dp + 4\tau_w \frac{dx}{D_h} = 0, \quad (C.31)$$

$$dh_0 = dh + V dV = 0. \quad (C.32)$$

Combining the second Gibbs equation ($Tds = dh - \frac{1}{\rho} dp$) with Eq. (C.32), then Eq. (C.31) gives:

$$ds = \frac{1}{\rho T} 4\tau_w \frac{dx}{D_h}. \quad (C.33)$$

The same Gibbs equation can then be used for an isentropic process to successively get:

$$dh_{is} = \frac{1}{\rho} dp, \quad \text{and} \quad ds = (\eta_{pol} - 1) \frac{1}{\rho T} dp, \quad (C.34)$$

C | An improved ejector thermodynamic model

Combining Eqs. (C.33) and (C.34), one obtains:

$$4\tau_w \frac{dx}{D_h} = (\eta_{pol} - 1) dp.$$

The momentum equation thus becomes:

$$\rho V dV + \eta_{pol} dp = 0. \quad (C.35)$$

The pressure differential can be expressed as:

$$dp = \left(\frac{\partial p}{\partial \rho} \right)_s d\rho + \left(\frac{\partial p}{\partial s} \right)_\rho ds. \quad (C.36)$$

The first partial derivative is the definition of the speed of sound squared whereas, the second partial derivative needs more development. In the case of an isentropic flow, the second term is obviously equal to zero. Using the first Gibbs equation ($Tds = \frac{R}{\gamma-1}dT + pd\left(\frac{1}{\rho}\right)$) along with the perfect gas assumption, one can write:

$$ds|_\rho = \frac{R}{(\gamma-1)} \frac{dT}{T},$$

$$\frac{dp|_\rho}{p} = \frac{dT}{T}.$$

Using these two expressions, the second partial derivative of Eq. (C.36) can be written as:

$$\left(\frac{\partial p}{\partial s} \right)_\rho = \frac{p(\gamma-1)}{R},$$

and Eq. (C.36), combined with Eq. (C.34) then becomes:

$$dp = \frac{a^2}{1 - (\eta_{pol} - 1)(\gamma - 1)} d\rho. \quad (C.37)$$

Relation between the compound-choking criterion and the maximization of the mass flow rate | 3.4

Combining this last expression with the momentum equation (C.35) and the mass conservation equation (C.30), one obtains:

$$\frac{dV}{V} \left(\frac{1 - (\eta_{pol} - 1)(\gamma - 1)}{\eta_{pol}} M^2 - 1 \right) = \frac{dA}{A}, \quad (C.38)$$

where the definition of the Mach number $M = \frac{V}{a}$ was used. The Mach number differential can be linked to the velocity differential by:

$$\frac{dV}{V} \left(1 + \frac{\gamma - 1}{2} M^2 \right) = \frac{dM}{M}, \quad (C.39)$$

and one can finally obtain the differential equation linking the Mach number to the cross-section area:

$$\frac{dM}{M} \frac{\frac{1 - (\eta_{pol} - 1)(\gamma - 1)}{\eta_{pol}} M^2 - 1}{1 + \frac{\gamma - 1}{2} M^2} = \frac{dA}{A}. \quad (C.40)$$

The throat is defined as the location in the nozzle where $dA = 0$ and this last equation shows that this will occur for a Mach number $M_t = \sqrt{\frac{\eta_{pol}}{\eta_{pol} + \gamma(1 - \eta_{pol})}}$ which is different from unity when $\eta_{pol} < 1$. This means that, as soon as the flow becomes non-isentropic, the flow does not reach sonic conditions at the throat when it is choked but somewhere further down the divergent. When the flow is considered to be non-isentropic, one can thus not use the unity Mach number at the throat as choking condition. This is in accordance with what was stated in Section 3.2.

3.4.2 Compound-choking criterion

One now considers a flow with several separate streams under the following assumptions:

1. The flow is one dimensional, steady-state and adiabatic.
2. There is no mixing between streams.
3. The pressure is constant between streams at each cross section.
4. The transverse pressure gradient caused by the streamline curvature is negligible.

C | An improved ejector thermodynamic model

Using the equations developed in the previous section, one can write, for each stream i :

$$\frac{dV_i}{V_i} \left(M_i^2 \frac{1 - (\eta_{pol,i} - 1)(\gamma_i - 1)}{\eta_{pol,i}} - 1 \right) = \frac{dA_i}{A_i}. \quad (C.41)$$

The momentum equation (C.35) expressed for each stream says that:

$$\rho_i V_i^2 \frac{dV_i}{V_i} = -\eta_{pol,i} dp_i, \quad (C.42)$$

$$\Rightarrow -\eta_{pol,i} \frac{dp_i}{\rho_i V_i^2} A_i \left(M_i^2 \frac{1 - (\eta_{pol,i} - 1)(\gamma_i - 1)}{\eta_{pol,i}} - 1 \right) = dA_i. \quad (C.43)$$

Since one considers that the pressure and thus the pressure differential is identical for all streams and that $\sum_i \frac{dA_i}{dx} = \frac{dA}{dx}$, one obtains:

$$\frac{1}{p} \frac{dp}{dx} \sum_i \frac{A_i}{\gamma_i M_i^2} \left(\eta_{pol,i} - M_i^2 (1 - (\eta_{pol,i} - 1)(\gamma_i - 1)) \right) = \frac{dA}{dx}. \quad (C.44)$$

One then defines the compound indicator β , similarly to what was done by Bernstein et al. [14], as:

$$\beta = \frac{\frac{dA}{dx}}{\frac{d(\ln(p))}{dx}}, \quad (C.45)$$

$$= \sum_i \frac{A_i}{\gamma_i M_i^2} \left(\eta_{pol,i} - M_i^2 (1 - (\eta_{pol,i} - 1)(\gamma_i - 1)) \right), \quad (C.46)$$

$$= \sum_i \frac{A_i}{\gamma_i} \left[\eta_{pol,i} \left(\frac{1}{M_i^2} - 1 \right) - \gamma_i (1 - \eta_{pol,i}) \right]. \quad (C.47)$$

This expression can be verified to match the expression from Bernstein et al. [14] for the case $\eta_{pol,i} = 1$. It can be shown through a compound wave analysis that this indicator must be equal to 0 for the compound flow to be choked.

Relation between the compound-choking criterion and the maximization of the mass flow rate | 3.4

3.4.3 Mass flow rate maximization for a supersonic ejector

From the compressible flow theory, when a flow is choked, its mass flow rate is maximized. Hence, if the compound-choking is the actual choking mechanism, it should be equivalent to maximizing the mass flow rate within the ejector. Since the primary mass flow rate is fixed, as the primary flow is itself choked in the primary nozzle, maximizing the mass flow rate in the ejector is equivalent to maximizing the secondary mass flow rate. The mass flow rate of the secondary flow in an ejector can be computed at the mixing section y using Eq. (C.12). Since the choking criteria (Fabri- or compound-choking) are destined at finding the pressure at the mixing section p_y such that the ejector is choked, the mass flow rate has to be maximized with respect to this pressure. One thus has:

$$\frac{\partial \dot{m}_s}{\partial p_y} = \frac{\dot{m}_s}{A_{s,y}} \left[\frac{1}{\rho_{s,y}} \frac{\partial \rho_{s,y}}{\partial p_y} A_{s,y} + \frac{1}{V_{s,y}} \frac{\partial V_{s,y}}{\partial p_y} A_{s,y} + \frac{\partial A_{s,y}}{\partial p_y} \right]. \quad (C.48)$$

The area of the secondary stream at the mixing section $A_{s,y}$ is not known a priori but since $A_y = A_{p,y} + A_{s,y}$, one has $\frac{\partial A_{s,y}}{\partial p_y} = -\frac{\partial A_{p,y}}{\partial p_y}$. Moreover, using the momentum equation (C.35), Eq. (C.48) becomes:

$$\frac{\partial \dot{m}_s}{\partial p_y} = \frac{\dot{m}_s}{A_{s,y}} \left[\frac{1}{\rho_{s,y}} \frac{\partial \rho_{s,y}}{\partial p_y} A_{s,y} - \frac{\eta_{pol,s}}{\rho_{s,y} V_{s,y}^2} A_{s,y} - \frac{\partial A_{p,y}}{\partial p_y} \right]. \quad (C.49)$$

Using the definition of the primary mass flow rate and the momentum equation (C.35), the last partial derivative of the previous equation can be written as:

$$\frac{\partial A_{p,y}}{\partial p_y} = A_{p,y} \left[-\frac{1}{\rho_{p,y}} \frac{\partial \rho_{p,y}}{\partial p_y} + \frac{\eta_{pol,p}}{\rho_{p,y} V_{p,y}^2} \right]. \quad (C.50)$$

Using this last relation as well as the link between the pressure and density differentials of Eq. (C.37), the derivative of the secondary mass flow rate with respect to the mixing pressure becomes:

$$\begin{aligned} \frac{\partial \dot{m}_s}{\partial p_y} = \frac{\dot{m}_s}{A_{s,y}} & \left[A_{s,y} \left(\frac{1 - (\eta_{pol,s} - 1)(\gamma_s - 1)}{\rho_{s,y} a_{s,y}^2} - \frac{\eta_{pol,s}}{\rho_{s,y} V_{s,y}^2} \right) \right. \\ & \left. + A_{p,y} \left(\frac{1 - (\eta_{pol,p} - 1)(\gamma_p - 1)}{\rho_{p,y} a_{p,y}^2} - \frac{\eta_{pol,p}}{\rho_{p,y} V_{p,y}^2} \right) \right], \end{aligned} \quad (C.51)$$

C | An improved ejector thermodynamic model

$$= \frac{\dot{m}_s}{A_{s,y} p_y} \left[\frac{A_{s,y}}{\gamma_s} \left(\eta_{pol,s} \left(1 - \frac{1}{M_{s,y}^2} \right) - \gamma_s (\eta_{pol,s} - 1) \right) + \frac{A_{p,y}}{\gamma_p} \left(\eta_{pol,p} \left(1 - \frac{1}{M_{p,y}^2} \right) - \gamma_p (\eta_{pol,p} - 1) \right) \right]. \quad (C.52)$$

This last expression can be compared to the expression of the compound-choking indicator β obtained in Eq. (C.47), taken for 2 streams at section y :

$$\frac{\partial \dot{m}_s}{\partial p_y} = - \frac{\dot{m}_s}{A_{s,y} p_y} \beta.$$

Thus it shows that applying the compound-choking criterion, i.e. $\beta = 0$ to an ejector is similar to maximizing the total mass flow rate within this ejector. More fundamentally, this shows that the choking mechanism at play in a supersonic ejector is the compound-choking. Indeed, the flow within a device is choked if the mass flow rate is maximized. Since maximizing the mass flow rate and applying the compound-choking criterion yield the same

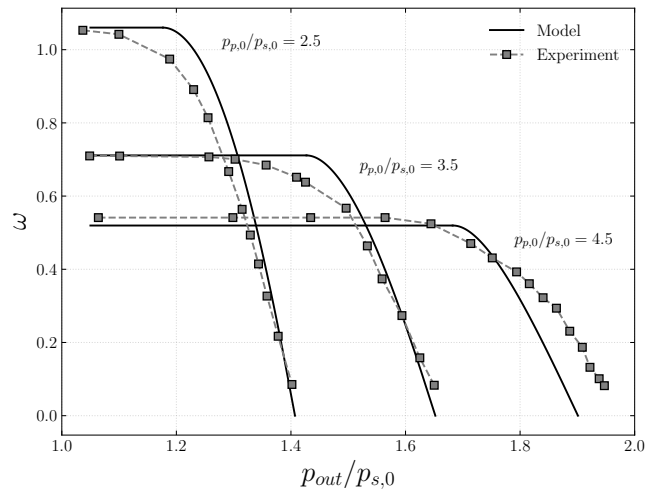


Fig. C.11 Corrected characteristic curves obtained for the air ejector test bench at Université catholique de Louvain with $\eta_p = 0.977$, $\eta_s = 0.71$ and $\eta_m = 0.95$. Comparison between the present thermodynamic model and new experimental data.

result, both must be equivalent. Building on this conclusion, it is possible to correct the previously obtained characteristic curves, that were spoiled by the spurious overshoot caused by the faulty application of the compound-choking criterion when dealing with non-isentropic transformations within the mixing chamber (Section 3.3). Figure C.11 shows the corrected version of the characteristic curves displayed in Figure C.10. Obtaining the corrected curves is actually rather straightforward, as one only needs to locate the maximum of the overshoot (in this case, in Fig. C.10), which indicates the location of the critical point and therefore of the on-design plateau. Note however that $\eta_s = 0.71$ in Figure C.11 for a better fitting of the experimental data.

3.5 Conclusion

In this paper, a new real gas thermodynamic model was presented. This model can be calibrated by means of multiple efficiencies. Although the model was only validated in the case of single-phase ejectors, it is foreseen to use this model for two-phase ejectors as well. This will be the subject of further studies.

First, a modified version of the model of Chen *et al.* [30] was implemented. As opposed to most models that can be found in the literature, this model uses the compound-choking criterion derived from the theory of Bernstein *et al.* [14], successfully applied to explain the choking mechanism in supersonic ejectors by Lamberts *et al.* [82, 85], and further developed in the frame of real gas ejectors by Fang [55] and Metsue [108]. Rather than assuming constant mixing pressure and using a variable mixing efficiency as in the model of Chen *et al.* [30], the mass conservation equation was re-introduced into the mixing model. The decrease in performance in the off-design regime is thereby modeled by pressure effects within the constant area duct. The new model was then used to perform an analysis on the connections between the Fabri-choking and the compound-choking. Despite the fact that the Fabri-choking seems to be the most straight-forward approach to model ejector entrainment limitation, it actually does not lead to the maximization of the mass flow rate within the device, which is in contradiction with the definition of a choked flow.

After the determination of the individual impact of each calibration parameter, the model was validated for single-phase R134a (ejectors of Garcia del Valle *et al.* [60] and Hakkaki-Fard *et al.* [71]) and air (ejector of Université catholique de Louvain) flows. A good fitting ability was obtained for both

C | An improved ejector thermodynamic model

fluids by using only three fitting parameters.

Lastly, an analytical study on the compound-choking criterion in the frame of non-isentropic perfect gas ejector flows showed that the use of the compound-choking criterion leads to the maximization of the total mass flow rate within the ejector. This is in accordance with the definition of choking for a simple nozzle (i.e. the maximization of the mass flow rate).

Future works include the validation of the present model for two-phase ejector predictions, especially those working with CO₂. The objective will be then to couple it to a model for a transcritical CO₂ heat pump and to assess the benefit of integrating an ejector on the performance of the whole cycle.



Investigation on Ejector Design for CO₂ Heat Pump Applications Using Dymola

The following work has been published in the proceedings of the 9th IIR Conference: Ammonia and CO₂ Refrigeration Technologies, and presented during the related event. It corresponds to reference [109].

4.1 Introduction

Ejectors are passive entrainment and compression devices that have a wide range of applications, going from desalination purposes [97] to waste heat recovery in thermal power plants [75]. Their main application resides however in refrigeration systems, where they are used as passive compressors; the high-pressure refrigerant is expanded into the ejector, which allows to suck and pre-compress the low-pressure refrigerant, thereby recovering part of the exergy losses associated with fluid expansion in a classical expansion valve. More details about the applications, functioning and modeling of supersonic ejectors may be found in the recent reviews of Besagni et al. [17], Ameer et al. [3, 4] and Tashtoush et al. [141].

Proper ejector design is crucial to allow for efficient heat pump systems.

D | Investigation of a CO₂ heat pump using dymola

As an example, experiments by Elbel and Hrnjak [51] showed that the presence of an ejector improves the coefficient of performance (COP) and the cooling capacity of the system by 7 and 8%, respectively. However, ejector design, especially for transcritical CO₂ heat pump systems, contains many challenges: lack of experimental data due to the difficulty of making measurements as CO₂ ejectors are small, transcritical nature of the flow as the primary flow flashes inside the primary nozzle, and difficulty to perform quality CFD computations due to their high computational cost. While appropriate CFDs are being developed for CO₂ ejectors, simplified models based on thermodynamic relations are often used as the main designing tool for ejectors. In the recent years, thermodynamic models, such as the models of Taslimi et al. [143] and Metsue et al. [110], have integrated increasingly more physics.

Performing in-house simulations of refrigeration cycles to design components may quickly become cumbersome, that is why modeling toolboxes such as Modelica are becoming more and more popular for such purposes [32, 67, 96, 92]. However, as such tools might allow one to quickly perform simulations, the components models remain quite limited regarding the physics they incorporate.

In this work, it is proposed to implement the state-of-the-art thermodynamic model of Metsue et al. [110], originally developed under Python, as a Dymola object and use it to investigate the ejector sizing influence on the performance of a transcritical CO₂ ejector heat pump cycle. First, the physical relevance of the two ejector models available in the TIL Modelica library, that is used as a basis for this work, is assessed. Then, the implementation of the model of Metsue et al. [110] into Modelica is shortly explained. The model is calibrated onto the experimental CO₂ data of Zhu et al. [155], and the resulting model is used to simulate the ejector heat pump cycle. Finally, results are discussed and the manuscript ends with the main conclusions and perspectives.

4.2 Limitations of TIL ejector models

Two models of ejector are available in the TIL library. The first model is based on the definition of a constant ejector efficiency η_{ej} , as defined by Elbel and Hrnjak [51]. The second one is based on an affinity relation between the pressure increase from the suction inlet and the suction mass flow rate. In order to highlight the limiting aspects of those two models, it is proposed to generate the characteristic curves. Figure D.1 compares the performance

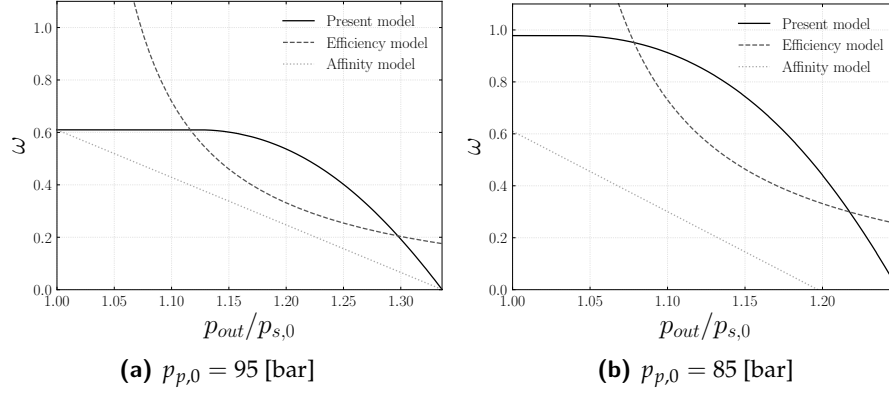


Fig. D.1 Comparison of the two ejectors models in TIL with the present model.

of the two aforementioned models, along with the in-house model at two primary inlet pressures. This latter model will be used, at this stage, for demonstration purposes only. Nevertheless, it has been calibrated for typical CO₂ heat pump applications and will serve as a reference in the following discussion. The operating conditions for the curves in Figure D.1 are listed in Table D.1. Both the Efficiency model and the Affinity model have been calibrated on the in-house model, at a primary pressure of 95 [bar]. As one may notice in Figure D.1a, the parameters of the Affinity model have been calibrated such that the zero pressure increase point and the breakdown pressure correspond to that of the in-house model. As for the efficiency-based model, the constant efficiency has been set to the mean of the ejector efficiency calculated with the in-house model. Curves presented in Figure D.1b have been plotted by keeping those same calibration parameters (for the three models), so that the only difference between Figure D.1a and Figure D.1b is the primary inlet pressure $p_{p,0}$. As shown in Figure D.1, none of the two TIL models are able to properly depict the process of double choking, i.e., the entrainment ratio plateau at low discharge pressures,

(a): $p_{p,0}$ [bar]	95	$T_{p,0}$ [°C]	35
(b): $p_{p,0}$ [bar]	85	$T_{s,0}$ [°C]	20
$p_{s,0}$ [bar]	35	A_t [m ²]	5.026×10^{-7}

Table D.1 Operating conditions.

and the rapid decrease in performance under the off-design regime. The entrainment ratio predicted by the Efficiency model reaches unrealistically high values as the discharge pressure is lowered, and fails to ever reach the breakdown point. This is easily explained by the fact that the ejector efficiency as defined in Elbel and Hrnjak [51] is not supposed to be constant with the discharge pressure. Rather, from its definition, η_{ej} should be a parabola-like function of the discharge pressure, equal to zero at the zero pressure increase point and breakdown point.

The Affinity model is better at modelling the decrease in ω , but there is still no distinction between on- and off-design regimes. In addition, note that both TIL models lack the ability to follow the physics when the inlet conditions change from nominal operation. As an example, Figure D.1b shows the predictions of the three models when the primary pressure is lowered by 10 [bar]. Most notably, the Affinity model then largely underestimates the entrainment ratio.

4.3 Ejector model implementation in dymola

As discussed in the previous subsection, the TIL ejector models, albeit being quite robust, do not include enough physics for ejector-centred and in-depth design studies. This motivates the implementation of a more advanced ejector model, that integrates more physics and geometrical parameters. To this end, the thermodynamic model of Mestue et al. [110], originally implemented in Python, is implemented into Dymola as a TIL object (i.e., using the VLEFluid classes and the TILMedia fluid properties provided by the library). As a short reminder, the model of Mestue et al. [110] is based on the maximization of the mass flow rates for single- and double-choking conditions. The ejector is discretized into several relevant sections, and the conservation equations, along with an isentropic efficiency equation, are

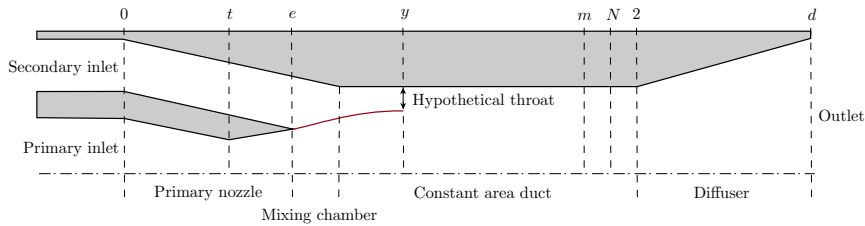


Fig. D.2 Schematic of the ejector model of Mestue et al. [110].

solved between each of those sections. Figure D.2 shows a schematic of the ejector. The interested reader may refer to Metsue *et al.* [110] for more details about the model.

Because Modelica is a modelling language, in contrast with traditional programming languages such as Python, the implementation of the model is not straightforward; some programming structures could not be re-implemented in Modelica and had to be re-thought. First, one must find the maximum mass flux G as a function of the primary pressure in order to solve the primary nozzle flow, which is impractical in Modelica as one cannot manipulate vectors. To solve this problem, the primary mass flux was implemented as a function of the primary pressure, and the flow was solved by adding Eq. D.1 to the system.

$$\frac{dG_t}{dp_p} = 0. \quad (\text{D.1})$$

Indeed, since $G(p_p)$ is a continuous and smooth function with a single maximum, finding the latter is equivalent to finding the zero of the derivative. For double choking operation, the same procedure has been implemented to find the maximum secondary mass flow rate as a function of the mixing pressure p_y :

$$\frac{d\dot{m}_s}{dp_y} = 0. \quad (\text{D.2})$$

Lastly, in order to assess the operating regime of the ejector, one should firstly calculate the on-design –critical– back pressure p_{out}^* . This is easily done in a conventional programming language, as one can compute said pressure as a first step and then, if the back pressure is higher than that, run the off-design part of the model. As a reminder, the ejector operates in off-design regime if:

$$p_{out} < p_{out}^*. \quad (\text{D.3})$$

However, in Dymola, the whole system of equation must be solved at each time step; one cannot simply choose which model to solve (on- or off-design). Therefore, the implemented ejector model contains an on-design ejector model within itself, which is disconnected from the main object inlets/outlet, and is only used to compute the on-design back pressure.

4.4 Calibration for CO₂ heat pump applications

To give plausible results, the model must be calibrated onto CO₂ data. As a reminder, the model of Metsue *et al.* [110] uses 5 efficiencies as calibration parameters ($\eta_p, \eta_s, \eta_{p,y}, \eta_m, \eta_d$). Note that the user also has to provide as inputs the main geometrical parameters of the ejector, that are, the primary nozzle throat and exit areas, as well as the mixing duct area.

For the present study, it was chosen to calibrate the model onto the experimental data of Zhu *et al.* [155]. Although the efficiencies should not be expected to be constant values, it was chosen, for the purpose of this work, to use one single set of efficiency values for all simulations. To this end, the model was fitted onto the experimental characteristic curve reported in [155] for $p_{p,0} = 93$ [bar]. Note that all other inlet conditions were kept constant, i.e., $p_{s,0} = 36$ [bar], $T_{p,0} = 35$ [°C] and $T_{s,0} = 21$ [°C].

Figure D.3 shows the result of the calibration process. One can see that it was possible to obtain a very good fitting for $p_{p,0} = 93$ [bar]. Keeping the same values for the efficiencies, the characteristic curves for $p_{p,0} = 87$ [bar] and $p_{p,0} = 98$ [bar] are also plotted. One may see that a good fitting is still obtained. Therefore, the set of efficiencies obtained through this calibration process will be used in the following sections.

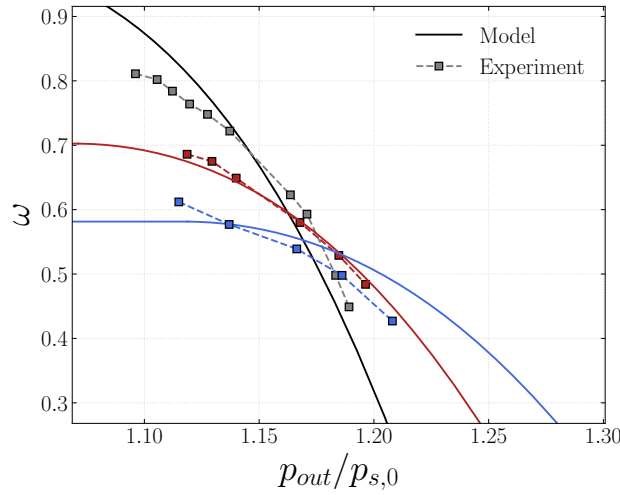


Fig. D.3 Fitting of the model onto the experimental data of Zhu *et al.* [155]. Blue: $p_{p,0} = 87$ [bar]; Red: $p_{p,0} = 93$ [bar]; Black: $p_{p,0} = 98$ [bar].

4.5 Investigation on ejector size

It is now proposed to investigate the influence of ejector size onto the performance of a transcritical CO₂ ejector heat pump cycle. To this end, the cycle presented in Figure D.4 is modeled. It consists of a three pressure levels air-water-heat pump. This kind of system is typically used to capture heat from ambient air and transfer it to a residence heating network to produce hot water.

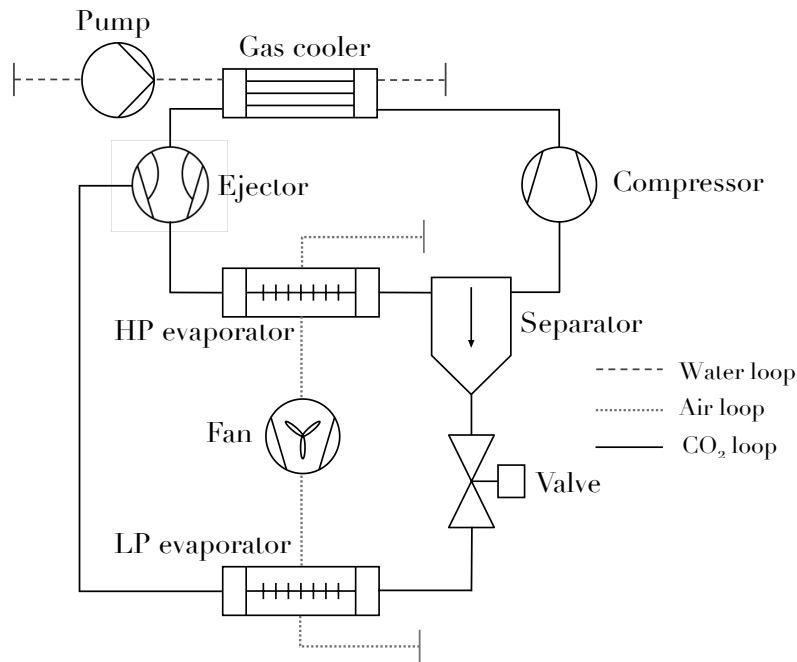


Fig. D.4 Schematic of the ejector-based heat pump cycle working with CO₂.

The present analysis stems from the hypothesis that there should exist an ejector size that best fits the system, i.e., that leads to the optimum COP. To verify this hypothesis, the ejector aspect ratio $AR = A_y / A_t$ (Figure D.2) is kept constant, whereas the ejector size (that is, A_t and A_y themselves) are varied. Note at this stage that the primary nozzle of the ejector of Zhu et al. [155] is convergent only, so that $A_t = A_e$. In addition, the compressor speed is regulated to maintain a hot water temperature of 65 [°C]. The main parameters for simulating this cycle are summarized in Table D.2. Figure

D | Investigation of a CO₂ heat pump using dymola

p_{water} [bar]	3	p_{amb} [bar]	1
T_{water} [°C]	65	T_{amb} [°C]	10
$\dot{m}_{pump}$ [kg.s ⁻¹]	3×10^{-2}	$\dot{V}_{fan}$ [m ³ .s ⁻¹]	1
D_{comp} [m ³]	10^{-5}	A_{valve} [m ²]	4×10^{-7}
V_{sep} [m ³]	2×10^{-3}	AR [-]	6.26

Table D.2 Main parameters for the simulation of the cycle.

D.5 shows the results as a function of the ejector size $A_t / A_{t,0}$, where $A_{t,0}$ is the nominal throat area that is used in the article of Zhu *et al.* [155]. Note that in order to obtain continuous curves, the ejector size was varied over a very long period of time, namely 10^5 [s], so that the system of equations becomes linear with time. As expected, there is a peak in performance for a particular value of the ejector size of $A_t / A_{t,0} \approx 0.55$ (Fig. D.5). Thus, one may actually improve the COP of the cycle by about 6.5% compared to the cycle using the original ejector size reported in Zhu *et al.* [155].

One may also observe in Figure D.5 that as the ejector gets bigger, the primary inlet pressure gets lower. Indeed, when the ejector size is increased, the primary mass flow rate increases. Thus, to maintain the same power transfer in the gas cooler, the density should be lower, which translates into decreases of both primary pressure and temperature. Furthermore, one

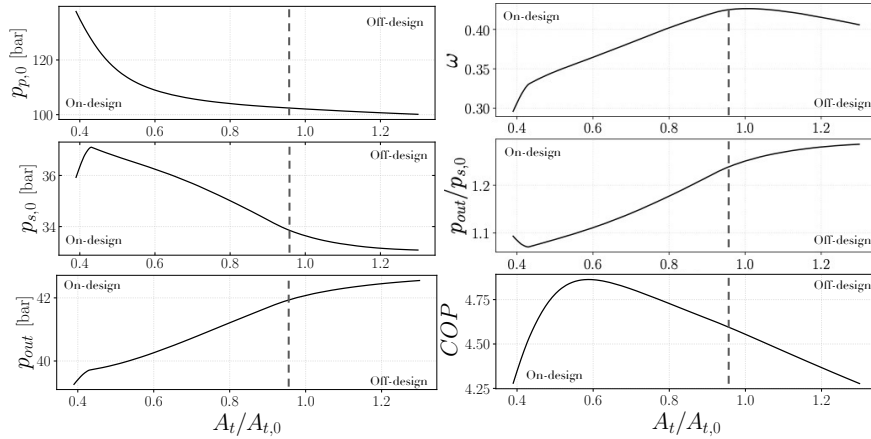


Fig. D.5 Ejector operating conditions and COP of the cycle as a function of the ejector size. The dashed line delimits on- and off-design regimes.

can observe that as the ejector size is increased, the discharge pressure gets higher, whereas the secondary inlet pressure gets lower, as a result of the flashing process in the expansion valve.

One might also mention the kink in the result curves for low ejector sizes. This is most likely due to the fact that at those operating conditions, the temperature at the CO₂ outlet of the gas cooler tends to reach the ambient temperature so that the power transfer potential from the CO₂ loop to the water loop becomes hindered by the small temperature pinch of the exchanger. This may be also attributed to the fact that the carbon dioxide mass flow rate through the gas cooler also gets smaller as the ejector becomes smaller. This translates into a shift in the cycle regime that one may observe at $A_t/A_{t,0} \approx 0.45$.

Lastly, it can be observed that there is no apparent correlation between the different performance parameters of the ejector and the cycle. This means that optimizing the cycle by optimizing the entrainment ratio or the compression ratio $p_{out}/p_{s,0}$ would not be the appropriate approach to design the ejector for a cycle such as the one presented in this work. Actually, the maximum ω point is found under off-design regime, and the compression ratio has no maximum. Note also that the critical ejector operation point –located at the on-off-design interface delimited by the dashed curve in Figure D.5– does not correspond to the maximum COP point. Instead, maximum cycle performance is found when the ejector is working well under on-design regime. This may in fact be a limitation of the present work, as one kept the ejector aspect ratio constant throughout this study. It might be possible to find an ejector geometry with even better performance –and at critical ejector operation– by varying A_t and A_y separately.

4.6 Conclusions

In this work, a state-of-the-art thermodynamic model has been implemented as a TIL object in the Dymola modeling tool. After proper calibration of said model, a transcritical CO₂ ejector heat pump system has been simulated. The study focused on the influence of the ejector size onto the performance of the global cycle.

First, it was found that the ready-to-use ejector models of Dymola were not representative of the ejector physics to the extent of the in-house model, which justifies its implementation. Then, the model was calibrated onto the experimental data of Zhu et al. [155], and a good overall fitting was

D | Investigation of a CO₂ heat pump using dymola

obtained over the range of experimental pressures.

Then, the ejector model was integrated into the heat pump system and the ejector size was varied. It was found that there was no apparent correlation between the ejector performance indicators and the coefficient of performance of the global cycle. Most notably, the optimum entrainment ratio of the ejector was found under the off-design regime, and the maximum coefficient of performance well under the on-design regime.

This work demonstrates that one should consider the whole cycle when performing ejector design, as an-ejector centered approach may not take the complex component dependencies into account. In addition, it must be noted that this study has been performed for a single ambient temperature, whereas real-life systems must obviously be regulated as the ambient conditions evolve. The optimum ejector size previously found is thus only valid for one operating point. Thus, it is foreseen to analyze the performance of more complex expansion devices such as multi-ejectors, as well as the performance with varying ambient conditions. Future work may also include the study of complex cycles such as booster cycles with parallel compression.

Bibliography

- [1] Flexi—Description and source code, 2023.
- [2] N. Abas, A. R. Kalair, N. Khan, A. Haider, Z. Saleem, and M. S. Saleem. Natural and synthetic refrigerants, global warming: A review. *Renewable and Sustainable Energy Reviews*, 90:557–569, 2018.
- [3] Z. Aidoun, K. Ameer, M. Falsafioon, and M. Badache. Current advances in ejector modeling, experimentation and applications for refrigeration and heat pumps. Part 1: Single-phase ejectors. *Inventions*, 4(1), 2019.
- [4] Z. Aidoun, K. Ameer, M. Falsafioon, and M. Badache. Current advances in ejector modeling, experimentation and applications for refrigeration and heat pumps. Part 2: Two-phase ejectors. *Inventions*, 4(1), 2019.
- [5] A. Ameli, A. Afzalifar, and T. Turunen-Saaresti. Non-equilibrium condensation of supercritical carbon dioxide in a converging-diverging nozzle. *Journal of Physics: Conference Series*, 821(012025):1–10, 2017.
- [6] K. Ameer, Z. Aidoun, and M. Ouzzane. Modeling and numerical approach for the design and operation of two-phase ejectors. *Applied Thermal Engineering*, 109:809 – 818, 2016.
- [7] W. Angielczyk, Y. Bartosiewicz, and D. Butrymowicz. Development of delayed equilibrium model for CO₂ convergent-divergent nozzle transonic flashing flow. *International Journal of Multiphase Flow*, 131(103351), 2020.
- [8] W. Angielczyk, Y. Bartosiewicz, D. Butrymowicz, and J.-M. Seynhaeve. 1-D modeling of supersonic carbon dioxide two-phase flow through

★ | Bibliography

ejector motive nozzle. In *International Refrigeration and Air Conditioning Conference*, pages 1–8, Purdue, 2010.

- [9] ANSYS. Ansys Fluent - CFD Software | ANSYS, 2023.
- [10] K. Banasiak, A. Hafner, E. E. Kriezi, K. B. Madsen, M. Birkelund, K. Fredslund, and R. Olsson. Development and performance mapping of a multi-ejector expansion work recovery pack for R744 vapour compression units. *International Journal of Refrigeration*, 57:265–276, 2015.
- [11] Y. Bartosiewicz, Z. Aidoun, P. Desevaux, and Y. Mercadier. Numerical and experimental investigations on supersonic ejectors. *International Journal of Heat and Fluid Flow*, 26(1):56–70, 2005.
- [12] Y. Bartosiewicz, Z. Aidoun, and Y. Mercadier. Numerical assessment of ejector operation for refrigeration applications based on CFD. *Applied Thermal Engineering*, 26(5):604–612, 2006.
- [13] I. H. Bell, J. Wronski, S. Quoilin, and V. Lemort. Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library CoolProp. *Industrial & Engineering Chemistry Research*, 53(6):2498–2508, 2014.
- [14] A. Bernstein, W. H. Heiser, and C. Hevenor. Compound-Compressible Nozzle Flow. *Journal of Applied Mechanics*, 34(3):548–554, 1967.
- [15] G. Besagni. Ejectors on the cutting edge: The past, the present and the perspective. *Energy*, 170:998–1003, 2019.
- [16] G. Besagni, N. Cristiani, L. Croci, G. R. Guédon, and F. Inzoli. Multi-scale evaluation of ejector performances: The influence of refrigerants and ejector design. *Applied Thermal Engineering*, 186:116502, 2021.
- [17] G. Besagni, R. Mereu, and F. Inzoli. Ejector refrigeration: A comprehensive review. *Renewable and Sustainable Energy Reviews*, 53:373–407, 2016.
- [18] Z. Bilicki, J. Kestin, and J. T. Stuart. Physical aspects of the relaxation model in two-phase flow. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 428(1875):379–397, 1990.

- [19] N. Bilir and H. K. Ersoy. Performance improvement of the vapour compression refrigeration cycle by a two-phase constant area ejector. *International Journal of Energy Research*, 33(5):469–480, 2009.
- [20] J. Bodys, M. Palacz, M. Haida, A. J. Nowak, and J. Smolka. Private communication, Feb. 2023.
- [21] J. Bodys, J. Smolka, M. Palacz, M. Haida, K. Banasiak, and A. J. Nowak. Effect of turbulence models and cavitation intensity on the motive and suction nozzle mass flow rate prediction during a non-equilibrium expansion process in the CO₂ ejector. *Applied Thermal Engineering*, 201:117743, 2022.
- [22] S. Bone. Comparative study of density-based versus pressure-based solvers for supersonic flow. Bachelor’s thesis, ETH Zürich, 2020.
- [23] A. Bouhanguel. *Etude numérique et expérimentale de l’interaction entre deux écoulements compressibles dans un éjecteur supersonique*. PhD thesis, Université de Franche-Comté, 2013.
- [24] A. Bouhanguel, P. Desevaux, and E. Gavignet. Flow visualization in supersonic ejectors using laser tomography techniques. *International Journal of Refrigeration*, 34(7):1633–1640, 2011.
- [25] A. Bouhanguel, P. Desevaux, and E. Gavignet. Visualization of flow instabilities in supersonic ejectors using large eddy simulation. *Journal of Visualization*, 18(1):17–19, 2015.
- [26] J. Bouré, A. Fritte, M. Giot, and M. Réocreux. Highlights of two-phase critical flow: On the links between maximum flow rates, sonic velocities, propagation and transfer phenomena in single and two-phase flows. *International Journal of Multiphase Flow*, 3(1):1–22, 1976.
- [27] S. Brown, S. Martynov, H. Mahgerefteh, S. Chen, and Y. Zhang. Modelling the non-equilibrium two-phase flow during depressurisation of CO₂ pipelines. *International Journal of Greenhouse Gas Control*, 30:9–18, 2014.
- [28] H. Bruce Stewart and B. Wendroff. Two-phase flow: Models and methods. *Journal of Computational Physics*, 56(3):363–409, 1984.
- [29] W. Chen, M. Liu, D. Chong, J. Yan, A. B. Little, and Y. Bartosiewicz. A 1D model to predict ejector performance at critical and sub-critical

★ | Bibliography

- operational regimes. *International Journal of Refrigeration*, 36(6):1750 – 1761, 2013.
- [30] W. Chen, C. Shi, S. Zhang, H. Chen, D. Chong, and J. Yan. Theoretical analysis of ejector refrigeration system performance under overall modes. *Applied Energy*, 185:2074 – 2084, 2017.
- [31] X. Chen, S. Omer, M. Worall, and S. Riffat. Recent developments in ejector refrigeration technologies. *Renewable and Sustainable Energy Reviews*, 19:629–651, 2013.
- [32] Y. Chen, Z. Chen, Z. Chen, and X. Yuan. Dynamic modeling of solar-assisted ground source heat pump using Modelica. *Applied Thermal Engineering*, 196:117324, 2021.
- [33] K. Cizungu, M. Groll, and Z.G. Ling. Modelling and optimization of two-phase ejectors for cooling systems. *Applied Thermal Engineering*, 25(13):1979 – 1994, 2005.
- [34] S. Croquer, Y. Fang, A. Metsue, Y. Bartosiewicz, and S. Poncet. Compound-choking theory for supersonic ejectors working with real gas. *Energy*, 227:120396, 2021.
- [35] S. Croquer, O. Lamberts, S. Poncet, S. Moreau, and Y. Bartosiewicz. Large eddy simulation of a supersonic air ejector. *Applied Thermal Engineering*, 209:118177, 2022.
- [36] S. Croquer, S. Poncet, and Z. Aidoun. Turbulence modeling of a single-phase R134a supersonic ejector. Part 1: Numerical benchmark. *International Journal of Refrigeration*, 61:140–152, 2016.
- [37] S. Croquer, S. Poncet, and Z. Aidoun. Thermodynamic modelling of supersonic gas ejector with droplets. *Entropy*, 19(11), 2017.
- [38] Q. Cui, C. Wang, E. Gao, and X. Zhang. Pinch point characteristics and performance evaluation of CO₂ heat pump water heater under variable working conditions. *Applied Thermal Engineering*, 207:118208, 2022.
- [39] C. Dang, K. Iino, and E. Hihara. Study on two-phase flow pattern of supercritical carbon dioxide with entrained pag-type lubricating oil in a gas cooler. *International Journal of Refrigeration*, 31:1265–1272, 11 2008.

- [40] M. De Lorenzo. *Modelling and numerical simulation of metastable two-phase flows*. PhD thesis, Université Paris Saclay, 2018.
- [41] M. De Lorenzo, P. Lafon, M. Di Matteo, M. Pelanti, J.-M. Seynhaeve, and Y. Bartosiewicz. Homogeneous two-phase flow models and accurate steam-water table look-up method for fast transient simulations. *International Journal of Multiphase Flow*, 95:199–219, 2017.
- [42] M. De Lorenzo, P. Lafon, J.-M. Seynhaeve, and Y. Bartosiewicz. Benchmark of delayed equilibrium model (DEM) and classic two-phase critical flow models against experimental data. *International Journal of Multiphase Flow*, 92:112–130, 2017.
- [43] R. Debroeyer, T. Toulorge, M. Rasquin, G. Winckelmans, , and Y. Bartosiewicz. Analysis of entrainment and mixing in a supersonic air ejector using large-eddy simulation. *International Journal of Heat and Fluid Flow [In review]*, 2024.
- [44] J.-Q. Deng, P.-X. Jiang, T. Lu, and W. Lu. Particular characteristics of transcritical CO₂ refrigeration cycle with an ejector. *Applied Thermal Engineering*, 27(2):381–388, 2007.
- [45] R. DiPippo. Chapter 8 - binary cycle power plants. In R. DiPippo, editor, *Geothermal Power Plants*, pages 193–239. Butterworth-Heinemann, Oxford, fourth edition, 2016.
- [46] P. Downar-Zapolski, Z. Bilicki, L. Bolle, and J. Franco. The non-equilibrium relaxation model for one-dimensional flashing liquid flow. *International Journal of Multiphase Flow*, 22(3):473–483, 1996.
- [47] J. L. Dupont, P. Domański, P. Lebrun, and F. Ziegler. The role of refrigeration in the global economy (2019). Technical report, International Institute of Refrigeration, 2019. 38th Note on Refrigeration Technologies.
- [48] V. Dvorak and P. Safarik. Supersonic flow structure in the entrance part of a mixing chamber of 2D model ejector. *Journal of Thermal Science*, 12(4):344–349, 2003.
- [49] I. W. Eames, S. Aphornratana, and H. Haider. A theoretical and experimental study of a small-scale steam jet refrigerator. *International Journal of Refrigeration*, 18(6):378 – 386, 1995.

★ | Bibliography

- [50] S. Elbel. Historical and present developments of ejector refrigeration systems with emphasis on transcritical carbon dioxide air-conditioning applications. *International Journal of Refrigeration*, 34(7):1545–1561, 2011.
- [51] S. Elbel and P. Hrnjak. Experimental validation of a prototype ejector designed to reduce throttling losses encountered in transcritical R744 system operation. *International Journal of Refrigeration*, 31(3):411–422, 2008.
- [52] S. Elbel and N. Lawrence. Review of recent developments in advanced ejector technology. *International Journal of Refrigeration*, 62:1–18, 2016.
- [53] ERTC. Constant area ejector, 2014.
- [54] J. Fabri and R. Siestrunck. Supersonic air ejectors. volume 5 of *Advances in Applied Mechanics*, pages 1 – 34. Elsevier, 1958.
- [55] Y. Fang. *Advanced numerical simulations of two-phase CO₂ ejectors*. PhD thesis, Université de Sherbrooke, 2019.
- [56] Y. Fang, M. De Lorenzo, P. Lafon, S. Poncet, and Y. Bartosiewicz. An accurate and efficient look-up table equation of state for two-phase compressible flow simulations of carbon dioxide. *Industrial & Engineering Chemistry Research*, 57(22):7676–7691, 2018.
- [57] Y. Fang, S. Poncet, H. Nesreddine, and Y. Bartosiewicz. An open-source density-based solver for two-phase CO₂ compressible flows: Verification and validation. *International Journal of Refrigeration*, 106:526–538, 2019.
- [58] S. Fangtian and M. Yitai. Thermodynamic analysis of transcritical CO₂ refrigeration cycle with an ejector. *Applied Thermal Engineering*, 31(6):1184–1189, 2011.
- [59] F. Föll, T. Hitz, C. Mueller, C.-D. Munz, and M. Dumbser. On the use of tabulated equations of state for multi-phase simulations in the homogeneous equilibrium limit. *Shock Waves*, 29:769–793, 07 2019.
- [60] J. García del Valle, J. Saíz Jabardo, F. Castro Ruiz, and J. San José Alonso. An experimental investigation of a R-134a ejector refrigeration system. *International Journal of Refrigeration*, 46:105 – 113, 2014.

- [61] J. García del Valle, J. Sierra-Pallares, P. Garcia Carrascal, and F. Castro Ruiz. An experimental and computational study of the flow pattern in a refrigerant ejector. Validation of turbulence models and real-gas effects. *Applied Thermal Engineering*, 89:795–811, 2015.
- [62] N. H. Gay. Refrigerating system, US patent US12490326A, Dec. 1931.
- [63] F. Giacomelli, F. Mazzelli, K. Banasiak, A. Hafner, and A. Milazzo. Experimental and computational analysis of a R744 flashing ejector. *International Journal of Refrigeration*, 107:326–343, 2019.
- [64] F. Giacomelli, F. Mazzelli, and A. Milazzo. Evaporation in supersonic CO₂ ejectors: analysis of theoretical and numerical models. In *9th International Conference on Multiphase Flow*, Firenze, 2016.
- [65] F. Giacomelli, F. Mazzelli, and A. Milazzo. A novel CFD approach for the computation of R744 flashing nozzles in compressible and metastable conditions. *Energy*, 162:1092–1105, 2018.
- [66] G. Grazzini, A. Milazzo, and F. Mazzelli. *Ejectors for Efficient Refrigeration: Design, Applications and Computational Fluid Dynamics*. Springer, 2018.
- [67] A. Hafner, S. Försterling, and K. Banasiak. Multi-ejector concept for R-744 supermarket refrigeration. *International Journal of Refrigeration*, 43:1–13, 2014.
- [68] M. Haida, M. Palacz, J. Bodys, J. Smolka, P. Gullo, and A. J. Nowak. An experimental investigation of performance and instabilities of the R744 vapour compression rack equipped with a two-phase ejector based on short-term, long-term and unsteady operations. *Applied Thermal Engineering*, 185:116353, 2021.
- [69] M. Haida, J. Smolka, A. Hafner, M. Mastrowski, M. Palacz, K. B. Madsen, A. J. Nowak, and K. Banasiak. Numerical investigation of heat transfer in a CO₂ two-phase ejector. *Energy*, 163:682–698, 2018.
- [70] M. Haida, J. Smolka, A. Hafner, M. Palacz, K. Banasiak, and A. J. Nowak. Modified homogeneous relaxation model for the R744 trans-critical flow in a two-phase ejector. *International Journal of Refrigeration*, 85:314–333, 2018.

★ | Bibliography

- [71] A. Hakkaki-Fard, Z. Aidoun, and M. Ouzzane. A computational methodology for ejector design and performance maximisation. *Energy Conversion and Management*, 105:1291 – 1302, 2015.
- [72] S. He, Y. Li, and R.Z. Wang. Progress of mathematical modeling on ejectors. *Renewable and Sustainable Energy Reviews*, 13(8):1760 – 1780, 2009.
- [73] A. Hemidi, F. Henry, S. Leclaire, J.-M. Seynhaeve, and Y. Bartosiewicz. CFD analysis of a supersonic air ejector. Part I: Experimental validation of single-phase and two-phase operation. *Applied Thermal Engineering*, 29(8):1523–1531, 2009.
- [74] B. J. Huang, J.M. Chang, C.P. Wang, and V.A. Petrenko. A 1-D analysis of ejector performance. *International Journal of Refrigeration*, 22(5):354 – 364, 1999.
- [75] O. Ipakchi, A. Mosaffa, and L. G. Farshi. Ejector based CO₂ transcritical combined cooling and power system utilizing waste heat recovery: A thermoeconomic assessment. *Energy Conversion and Management*, 186:462 – 472, 2019.
- [76] M. R. Islam. Chapter 7 - field guidelines. In M. R. Islam, editor, *Reservoir Development*, Sustainable Oil and Gas Development Series, pages 737–843. Gulf Professional Publishing, 2022.
- [77] J. H. Keenan, E. P. Neumann, and F. Lustwerk. An investigation of ejector design by analysis and experiment. *Journal of Applied Mechanics*, 17(3):299–309, 1950.
- [78] A. Khosravi, R.N.N. Koury, and L. Machado. Thermo-economic analysis and sizing of the components of an ejector expansion refrigeration system. *International Journal of Refrigeration*, 86:463–479, 2018.
- [79] M.-H. Kim, J. Pettersen, and C. W. Bullard. Fundamental process and system design issues in CO₂ vapor compression systems. *Progress in Energy and Combustion Science*, 30(2):119–174, 2004.
- [80] A. A. Kornhauser. The use of an ejector as a refrigerant expander. In *International Refrigeration and Air Conditioning Conference*, Purdue, 1990.

- [81] E. B. Ksayer and D. Clodic. Enhancement of CO₂ refrigeration cycle using an ejector: 1D analysis. In *11th International Refrigeration and Air-Conditioning Conference*, Purdue, 2006.
- [82] O. Lamberts. *Choking and mixing phenomena in supersonic ejectors*. PhD thesis, Université Catholique de Louvain, 2018.
- [83] O. Lamberts, P. Chatelain, and Y. Bartosiewicz. New methods for analyzing transport phenomena in supersonic ejectors. *International Journal of Heat and Fluid Flow*, 64:23–40, 2017.
- [84] O. Lamberts, P. Chatelain, and Y. Bartosiewicz. Numerical and experimental evidence of the Fabri-choking in a supersonic ejector. *International Journal of Heat and Fluid Flow*, 69:194 – 209, 2018.
- [85] O. Lamberts, P. Chatelain, N. Bourgeois, and Y. Bartosiewicz. The compound-choking theory as an explanation of the entrainment limitation in supersonic ejectors. *Energy*, 158:524 – 536, 2018.
- [86] E. W. Lemmon, M. L. Huber, and M. O. McLinden. *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties - REFPROP*. Gaithersburg, 9.0 edition, 2010.
- [87] D. Li and E. A. Groll. Transcritical CO₂ refrigeration cycle with ejector-expansion device. *International Journal of Refrigeration*, 28(5):766–773, 2005.
- [88] H. Li, F. Cao, X. Bu, L. Wang, and X. Wang. Performance characteristics of R1234yf ejector-expansion refrigeration cycle. *Applied Energy*, 121:96–103, 2014.
- [89] Y. Li and J. Deng. Numerical investigation on the performance of transcritical CO₂ two-phase ejector with a novel non-equilibrium CFD model. *Energy*, 238:121995, 2022.
- [90] Y. Li, J. Deng, L. Ma, and Y. Zhang. Visualization of two-phase flow in primary nozzle of a transcritical CO₂ ejector. *Energy Conversion and Management*, 171:729–741, 2018.
- [91] A. B. Little and S. Garimella. A critical review linking ejector flow phenomena with component- and system-level performance. *International Journal of Refrigeration*, 70:243–268, 2016.

★ | Bibliography

- [92] F. Liu, J. Deng, and W. Pan. Model-based dynamic optimal control of an ejector expansion CO₂ heat pump coupled with thermal storages. *Energy Procedia*, 152:156–161, 2018.
- [93] F. Liu, E. A. Groll, and D. Li. Investigation on performance of variable geometry ejectors for CO₂ refrigeration cycles. *Energy*, 45(1):829–839, 2012.
- [94] F. Liu, Y. Li, and E. A. Groll. Performance enhancement of CO₂ air conditioner with a controllable ejector. *International Journal of Refrigeration*, 35(6):1604–1616, 2012.
- [95] F. Liu, H. Liu, Y. Liu, G. Yu, X. Zhao, Y. Fan, C. Peng, and Q. Li. Transient numerical study of CO₂ two-phase flow in a needle adjustable ejector. *International Journal of Heat and Mass Transfer*, 214:124395, 2023.
- [96] F. Liu, W. Qiu, J. Deng, Q. Mo, E. A. Groll, J. Zhao, and J. Liang. Multi-objective non-simultaneous dynamic optimal control for an ejector expansion heat pump with thermal storages. *Applied Thermal Engineering*, 168:114835, 2020.
- [97] J. Liu, L. Wang, L. Jia, and H. Xue. Thermodynamic analysis of the steam ejector for desalination applications. *Applied Thermal Engineering*, 159:113883, 2019.
- [98] A. M. Log, M. Hammer, H. Deng, A. Austegard, A. Hafner, and S. T. Munkejord. Depressurization of CO₂ in a pipe: Effect of initial state on non-equilibrium two-phase flow. *International Journal of Multiphase Flow*, 170:104624, 2024.
- [99] A. M. Log, M. Hammer, and S. T. Munkejord. A flashing flow model for the rapid depressurization of CO₂ in a pipe accounting for bubble nucleation and growth. *International Journal of Multiphase Flow*, 171:104666, 2024.
- [100] J. Long, B. Yu, D. Wang, C. Liu, J. Shi, and J. Chen. A novel relaxation drift model for simulating liquid-vapor momentum non-equilibrium in two-phase ejectors. *Case Studies in Thermal Engineering*, 52:103758, 2023.
- [101] M. A. Lopez de Bertodano. Two fluid model for two-phase turbulent jets. *Nuclear Engineering and Design*, 179(1):65–74, 1998.

- [102] C. Lucas and J. Koehler. Experimental investigation of the COP improvement of a refrigeration cycle by use of an ejector. *International Journal of Refrigeration*, 35(6):1595–1603, 2012.
- [103] C. Lucas, H. Rusche, A. Schroeder, and J. Koehler. Numerical investigation of a two-phase CO₂ ejector. *International Journal of Refrigeration*, 43:154–166, 2014.
- [104] H. Lund, T. Flåtten, and S. T. Munkejord. Depressurization of carbon dioxide in pipelines—models and methods. *Energy Procedia*, 4:2984–2991, 2011.
- [105] M. Manninen, V. Taivassalo, and S. Kallio. On the mixture model for multiphase flow. *VTT Publications*, 288:1–67, 1996.
- [106] F. Mazzelli, A. B. Little, S. Garimella, and Y. Bartosiewicz. Computational and experimental analysis of supersonic air ejector: Turbulence modeling and assessment of 3D effects. *International Journal of Heat and Fluid Flow*, 56:305–316, 2015.
- [107] F. R. Menter. Zonal two equation $k-\omega$ turbulence models for aerodynamic flows. In *23rd Fluid Dynamics, Plasmadynamics, and Lasers Conference*, Orlando, USA, 1993.
- [108] A. Metsue. An improved thermodynamic model for supersonic ejectors. Master’s thesis, Université catholique de Louvain, 2020.
- [109] A. Metsue, Y. Bartosiewicz, and S. Poncet. Investigation on ejector design for CO₂ heat pump applications using Dymola. In *Proc. of the 9th IIR International Conference Ammonia and CO₂ Refrigeration Technologies*, pages 211–218, Ohrid, 2021.
- [110] A. Metsue, R. Debroeyer, S. Poncet, and Y. Bartosiewicz. An improved thermodynamic model for supersonic real-gas ejectors using the compound-choking theory. *Energy*, 238:121856, 2022.
- [111] A. Metsue, H. Nesreddine, Y. Bartosiewicz, and S. Poncet. Theoretical analysis of the optimal ejector operation and design within an ejector-based refrigeration system. *Submitted to the International Journal of Refrigeration*, 2024.
- [112] A. Metsue, H. Nesreddine, D. Monney, Y. Bartosiewicz, and S. Poncet. Simulation and exergy analysis of transcritical CO₂ ejectors flows

using the implicit real gas SU2 solver. In *26th IIR International Congress of Refrigeration*, volume 2, pages 939–950, Paris, 2023.

- [113] A. Metsue, S. Poncet, and Y. Bartosiewicz. A homogeneous relaxation model algorithm in density-based formulation with novel tabulated method for the modeling of CO₂ flashing nozzles. *International Journal of Refrigeration*, 161:188–201, 2024.
- [114] J. Meyers and C. Meneveau. Flow visualization using momentum and energy transport tubes and applications to turbulent flow in wind farms. *Journal of Fluid Mechanics*, 715:335–358, 2013.
- [115] A. Morin, P. Aursand, T. Flåtten, and S. T. Munkejord. Numerical resolution of CO₂ transport dynamics. In *2009 SIAM Conference on Mathematics for Industry*, San Francisco, 2009.
- [116] J. T. Munday and D. F. Bagster. A new ejector theory applied to steam jet refrigeration. *Industrial & Engineering Chemistry Process Design and Development*, 16(4):442–449, 1977.
- [117] M. Nakagawa, M. S. Berana, and A. Kishine. Supersonic two-phase flow of CO₂ through converging–diverging nozzles for the ejector refrigeration cycle. *International Journal of Refrigeration*, 32(6):1195–1202, 2009.
- [118] E. Nehdi, L. Kairouani, and M. Bouzaina. Performance analysis of the vapour compression cycle using ejector as an expander. *International Journal of Energy Research*, 31(4):364–375, 2007.
- [119] F. Palacios, M. Colonno, A. Aranake, A. Campos, S. Copeland, T. Economon, A. Lonkar, T. Lukaczyk, T. Taylor, and J. Alonso. Stanford university unstructured (SU2): An open-source integrated computational environment for multi-physics simulation and design. In *51st AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition 2013*, 2013.
- [120] M. Palacz, J. Bodys, M. Haida, J. Smolka, and A. J. Nowak. Two-phase flow visualisation in the R744 vapour ejector for refrigeration systems. *Applied Thermal Engineering*, 210:118322, 2022.
- [121] M. Palacz, M. Haida, J. Smolka, A. J. Nowak, K. Banasiak, and A. Hafner. HEM and HRM accuracy comparison for the simulation

of CO₂ expansion in two-phase ejectors for supermarket refrigeration systems. *Applied Thermal Engineering*, 115:160–169, 2017.

- [122] M. Palacz, J. Smolka, A. Fic, Z. Bulinski, A. J. Nowak, K. Banasiak, and A. Hafner. Application range of the HEM approach for CO₂ expansion inside two-phase ejectors for supermarket refrigeration systems. *International Journal of Refrigeration*, 59:251–258, 2015.
- [123] G. Pottker and P. Hrnjak. Ejector in R410A vapor compression systems with experimental quantification of two major mechanisms of performance improvement: Work recovery and liquid feeding. *International Journal of Refrigeration*, 50:184–192, 2015.
- [124] D. Quinn, D. Stannard, J. Edwards, K. K. Botros, and C. Johansen. Experimental visualization and characteristics of bubble nucleation during rapid decompression of supercritical and subcooled carbon dioxide. *International Journal of Pressure Vessels and Piping*, 195:104569, 2022.
- [125] M. R. Rahamathullah, P. Karthick, T. Aridas, V. Prabakaran, Sathiamourthy, and P. Sarangapani. A review on historical and present developments in ejector systems. *International Journal of Engineering Research and Applications*, 3(2):10–34, 2013.
- [126] S. K. Raman and H.D. Kim. Solutions of supercritical CO₂ flow through a convergent-divergent nozzle with real gas effects. *International Journal of Heat and Mass Transfer*, 116:127–135, 2018.
- [127] S. Rao and J. Gopalan. Observations on the non-mixed length and unsteady shock motion in a two dimensional supersonic ejector. *Physics of Fluids*, 26:036103, 2014.
- [128] S. B. Riffat and S. A. Omer. CFD modelling and experimental investigation of an ejector refrigeration system using methanol as the working fluid. *International Journal of Energy Research*, 25(2):115–128, 2001.
- [129] K. E. Ringstad, Y. Allouche, P. Gullo, A. Ervik, K. Banasiak, and A. Hafner. A detailed review on CO₂ two-phase ejector flow modeling. *Thermal Science and Engineering Progress*, 20:100647, 2020.
- [130] P. Roe. Approximate Riemann solvers, parameter vectors, and difference schemes. *Journal of Computational Physics*, 43(2):357–372, 1981.

★ | Bibliography

- [131] E. D. Rogdakis and G.K. Alexis. Design and parametric investigation of an ejector in an air-conditioning system. *Applied Thermal Engineering*, 20(2):213 – 226, 2000.
- [132] A. Rubino, M. Pini, M. Kosec, S. Vitale, and P. Colonna. A look-up table method based on unstructured grids and its application to non-ideal compressible fluid dynamic simulations. *Journal of Computational Science*, 28:70–77, 2018.
- [133] J. Sarkar. Geometric parameter optimization of ejector-expansion refrigeration cycle with natural refrigerants. *International Journal of Energy Research*, 34(1):84–94, 2010.
- [134] M. Scott and D. Kyritsis. Quantitative visualization of CO₂-oil mixtures in CO₂ expansion flows. Technical report, Air Conditioning and Refrigeration Center TR-255, University of Illinois at Urbana-Champaign, 2007.
- [135] A. Selvaraju and A. Mani. Analysis of an ejector with environment friendly refrigerants. *Applied Thermal Engineering*, 24(5):827 – 838, 2004.
- [136] A. H. Shapiro. *The Dynamics and thermodynamics of compressible fluid flow: The Dynamics and thermodynamics of compressible fluid flow*. Ronald, 1953.
- [137] S. A. Sherif, W.E. Lear, J.M. Steadham, P.L. Hunt, and J.B. Holladay. Analysis and modeling of a two-phase jet pump of a thermal management system for aerospace applications. *International Journal of Mechanical Sciences*, 42(2):185 – 198, 2000.
- [138] S. Singh, A. Hafner, M.P. Maiya, K. Banasiak, and P. Neksa. Multi-ejector CO₂ cooling system with evaporative gas cooler for a supermarket application in tropical regions. *Applied Thermal Engineering*, 190(116766), 2021.
- [139] J. Smolka, Z. Bulinski, A. Fic, A. J. Nowak, K. Banasiak, and A. Hafner. A computational model of a transcritical R744 ejector based on a homogeneous real fluid approach. *Applied Mathematical Modelling*, 37(3):1208–1224, 2013.
- [140] R. Span and W. Wagner. A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K

at pressures up to 800 MPa. *Journal of Physical and Chemical Reference Data*, 25(6):1509–1596, 1996.

- [141] B. M. Tashtoush, M. A. Al-Nimr, and M. A. Khasawneh. A comprehensive review of ejector design, performance, and applications. *Applied Energy*, 240:138–172, 2019.
- [142] S. Taslimi Taleghani, M. Sorin, and S. Poncet. Energy and exergy efficiencies of different configurations of the ejector-based CO₂ refrigeration systems. *International Journal of Energy Production and Management*, 3(1):22–33, 2018.
- [143] S. Taslimi Taleghani, M. Sorin, and S. Poncet. Modeling of two-phase transcritical CO₂ ejectors for on-design and off-design conditions. *International Journal of Refrigeration*, 87:91 – 105, 2018.
- [144] United Nations Environment Programme (UNEP). Kigali amendment to the montreal protocol. Amendment adopted at the 28th Meeting of the Parties to the Montreal Protocol, 2016. Available online: <https://ozone.unep.org/treaties/montreal-protocol/amendments/>.
- [145] J. Van den Berghe, J. Vemula, Y. Bartosiewicz, and M. Mendez. A machine learning-based calibration of a 1D ejector model from CFD. In *36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems*, pages 424–435, Las Palmas de Gran Canaria, 2023.
- [146] K. Wang, L. Wang, and R. Gao. An extended mechanism model of gaseous ejectors. *Energy*, 264:126094, 2023.
- [147] R. L. Yadav and A. W. Patwardhan. Design aspects of ejectors: Effects of suction chamber geometry. *Chemical Engineering Science*, 63(15):3886–3897, 2008.
- [148] J. Yan, N. Wen, L. Wang, X. Li, Z. Liu, and S. Li. Optimization on ejector key geometries of a two-stage ejector-based multi-evaporator refrigeration system. *Energy Conversion and Management*, 175:142–150, 2018.
- [149] M. Zegenhagen and F. Ziegler. A one-dimensional model of a jet-ejector in critical double choking operation with R134a as a refrigerant including real gas effects. *International Journal of Refrigeration*, 55:72–84, 2015.

★ | Bibliography

- [150] H. Zeng, H. Zhao, H. Zhang, and Z. Liu. Simulation study of key cross-sectional area dimensions of CO₂ ejector on performance. *International Journal of Refrigeration*, 159:276–286, 2024.
- [151] Z. Zhang and L. Tian. Effect of suction nozzle pressure drop on the performance of an ejector-expansion transcritical CO₂ refrigeration cycle. *Entropy*, 16(8):4309–4321, 2014.
- [152] L. Zhao, X. Yang, S. Deng, H. Li, and Z. Yu. Performance analysis of the ejector-expansion refrigeration cycle using zeotropic mixtures. *International Journal of Refrigeration*, 57:197–207, 2015.
- [153] L. Zheng, J. Deng, Y. He, and P. Jiang. Dynamic model of a transcritical CO₂ ejector expansion refrigeration system. *International Journal of Refrigeration*, 60:247–260, 2015.
- [154] J. Zhu, F. Botticella, and S. Elbel. Experimental investigation and theoretical analysis of oil circulation rates in ejector cooling cycles. *Energy*, 157:718–733, 2018.
- [155] Y. Zhu, C. Li, F. Zhang, and P.-X. Jiang. Comprehensive experimental study on a transcritical CO₂ ejector-expansion refrigeration system. *Energy Conversion and Management*, 151:98–106, 2017.
- [156] Y. Zhu, Z. Wang, Y. Yang, and P.-X. Jiang. Flow visualization of supersonic two-phase transcritical flow of CO₂ in an ejector of a refrigeration system. *International Journal of Refrigeration*, 74:354–361, 2017.