METASTABILITY EFFECTS IN THE PHASE TRANSITION PROCESSES FOR TRANSCRITICAL R744 CONVERGING-DIVERGING NOZZLES

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ABSTRACT

The metastability effects in the phase transition processes for transcritical R744 converging-diverging nozzles were investigated in this study. The research comprised both numerical simulations and experimental measurements, performed over the range of operating conditions typical for a heat pump. The nozzle model utilized the Delayed Equilibrium Model supplied with the nucleation approach based on a superposition of homogeneous and heterogeneous nucleation. The experimental investigation was performed at the test facility for the analysis of expansion work recovery ejectors in small-scale heat pumps. Based on results of the experimental tests for conical geometries, the authors first developed than validated the correlation equation for the nucleation work reduction factor for a typical range of operating conditions. The absolute values of the relative errors between the simulation and the experimental results for the critical mass flux were acceptably low.

1. INTRODUCTION

The research effort on the R744 converging-diverging nozzles reported in the literature is substantial and comprises both experimental work and numerical simulations, however the field is far from being thoroughly examined. Nakagawa et al. (2009) experimentally investigated the supersonic two-phase flow of R744 in the diverging sections of rectangular converging–diverging nozzles for inlet temperatures from 20 °C to 37 °C and inlet pressures from 6 MPa to 9 MPa. Based on the results obtained, the authors advanced into the analysis of shock wave propagation in the supersonic R744 liquid-vapor flows for the same type of motive nozzle, Berana et al. (2009). Based on the results by Nakagawa et al. (2009), Angielczyk et al. (2010) utilized the Homogeneous Relaxation Model (HRM) for 1D nozzle modeling. The authors simulated the decompression curves for the selected nozzle geometry and boundary conditions and obtained reasonable matching. However, the limited amount of reference data made reliable validation of the presented mathematical model impossible.

Banasiak and Hafner (2011) presented a one-dimensional model of the R744 two-phase ejector, in which the Delayed Equilibrium Model (DEM), Attuo and Seynhaeve (1999), for a transcritical flow with delayed flashing over the motive nozzle was utilized. The authors validated the motive nozzle model for the critical mass flow rate for a typical range of operating conditions and obtained a relative deviation within the range of ±5%. However, the authors arbitrarily assumed the homogeneous nucleation to be the sole flashing mechanism, which actually deviates from real cases, where the metastable fluid is surrounded by walls that contain cavities acting as nucleation sites. The heterogeneous nucleation effect should be considered, especially for evaporation pressures that are considerably below the critical point, Gerum et al. (1979).

For that reason, the main objective of this study was to analyze the effects of various approaches for phase transition on the results of numerical simulations of transcritical R744 expansion in the ejector motive nozzle. The computational work was performed by means of the authors' own mathematical model, Banasiak and Hafner (2011), while the measurements were collected at the specially designed ejector-equipped test facility.

2. PHASE TRANSITION APPROACHES

The thermodynamic state of a two-phase fluid was modeled by the DEM approach, where the variable called 'vaporization index', denoting the mass fraction of the fluid transformed into a saturated mixture of vapor and liquid, was introduced as an additional variable, Attuo, and Seynhaeve (1999). This approach requires an additional closure equation for the vaporization index, expressed as a function of the vapor generation rate.

In the classic nucleation theory, the mass generation rate during the non-equilibrium phase change process is given by the sum of the mass increase due to nucleation (the formation of critically sized bubbles/droplets) and the growth/demise of the formed globules, according to Ishazaki et al. (1995). The nucleation rate, dependent on the phase transition approach, may be considered as follows:

- infinitesimally large for the Homogeneous Equilibrium Model (HEM),
- governed by spontaneous molecular fluctuations in bulk liquid only for homogeneous nucleation,
- governed by molecular fluctuations promoted in cavities of the wall surface only for heterogeneous nucleation,
- ruled by both nucleation mechanisms for a superposition of the last two modes,

where the last approach is highly recommended for the mathematical modeling of nucleation and flashing in adiabatic ducts, Kolev (2007).

The homogeneous nucleation is determined solely by fluid properties and actual superheat/subcooling, while the heterogeneous nucleation mechanism involves two additional effects: the influence of the walls' structure, which is usually expressed by surface roughness, and the molecular interaction between solid and liquid, which is usually characterized by the parameter called the contact angle. Thus, most common correlations for the nucleation rate are expressed as functions of superheat/subcooling, contact angle, duct geometry, and additional variable φ, referred to as the nucleation work reduction factor, Kolev (2007), or the ratio of activation energies, Gerum et al. (1979). This parameter denotes the ratio of the nucleation energy required for the creation of bubbles at the walls to the energy required for the creation of bubbles in a bulk liquid for the same superheat/subcooling. Its values are confined between 0 and 1, and depend significantly on the nucleation site density and shape, the depressurization speed, and the phase transition pressure level. Because numerous theoretical models of the heterogeneous nucleation kinetics yielded results that deviated significantly from the real cases, experimental tests remain the most efficient method for determining values of φ, Kolev (2007).

For flashing flows, the higher the nucleation rate, the lower the critical mass flow rate, due to significantly reduced speed of sound for the two-phase region. As a consequence, based on the measured values of the critical mass flow rate for a given nozzle, by means of solving an inverse problem it is possible to find values of φ that could match the results of numerical simulations to the results of experimental tests.

Therefore, for the purpose of this research, the authors of the paper applied an approach based on the superposition of homogeneous and heterogeneous nucleation for phase transition modeling and investigated the work reduction factor values for the R744 flow through a conically shaped, stainless steel converging-diverging nozzle based on the results of experimental measurements.

3. EXPERIMENTAL SETUP

All of the experiments were performed at a specially designed facility for ejector testing at the SINTEF Energi laboratory in Trondheim, Figure 1. The ejector assembly consisted of 4 main body parts: the motive/suction nozzle section, the mixing section, the diffuser section, and the ending section. The measurement system was based on temperature sensors (calibrated T-type thermocouples, uncertainty equal to ±0.5 K), absolute and differential pressure sensors (calibrated piezoelectric elements, uncertainty equal to $\pm 30\times10^3$ Pa), and mass flow meters (calibrated Coriolis type, uncertainty equal to ±0.0005 kg/s).

The tests were performed for 5 optional geometry variants of the motive nozzle. The main construction parameters were listed in Table 1.

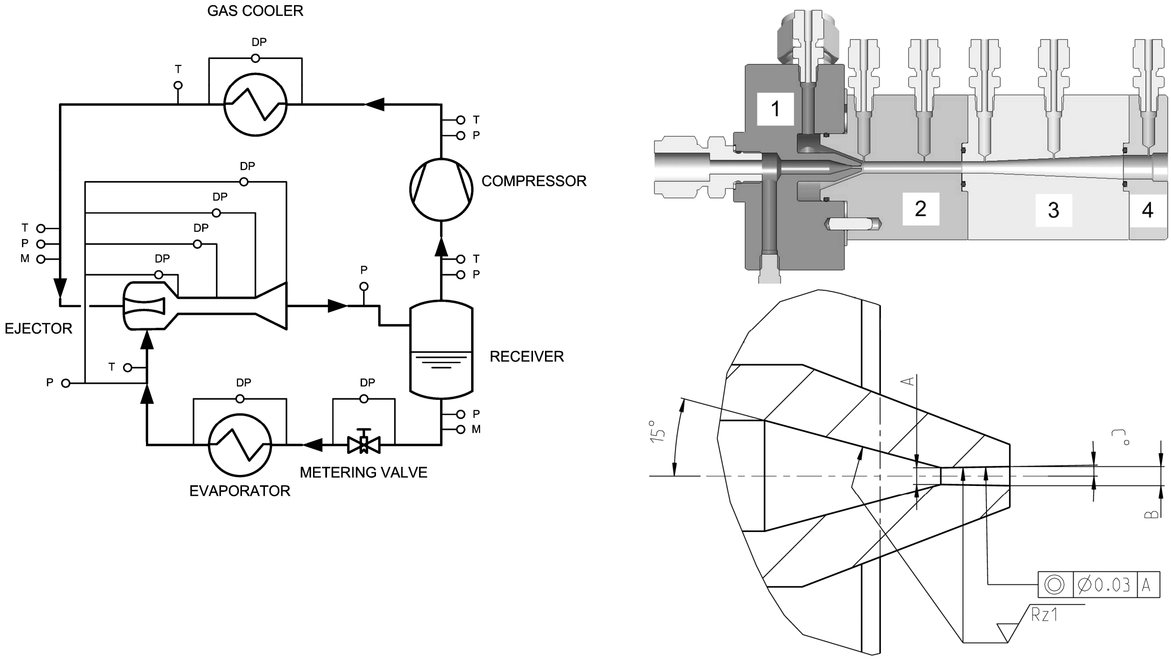


Figure 1. Schematics of the R744 ejector test facility (on the left) and ejector assembly and basic dimensions of the motive nozzle (on the right). T - temperature sensor, P - absolute pressure sensor, DP - differential pressure sensor, M - mass flow rate meter. 1 – the nozzle section, 2 – the mixing section, 3 – the diffuser section, 4 – the ending section. The motive nozzle inlet diameter was 6×10-3 m for all geometry variants, dimensions (A), (B), and (C), according to Table 1.

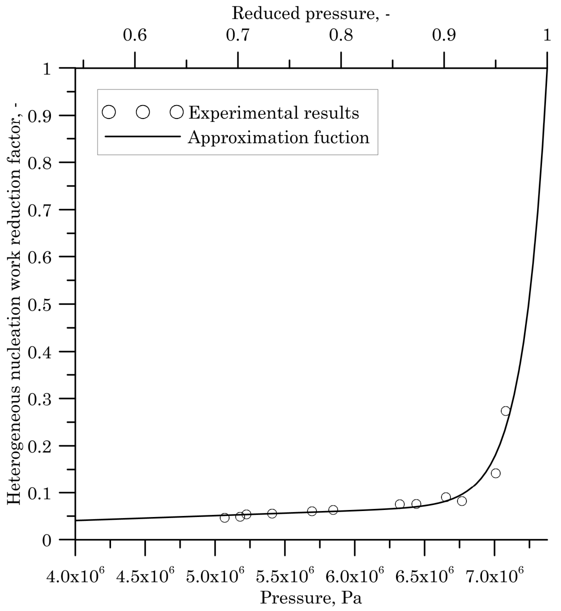
Table 1. Motive nozzle geometry variants for the validation procedure (the dimension notation referenced in Figure 1).

Nozzle signature	**N1**	**N2**	**N3**	**N4**	**N5**
A, 10^{-3} m	0.91	1.21	1.41	1.58	1.2
B, 10^{-3} m	1.02	1.33	1.53	1.73	1.2
C, °	0.92	1	1	1	0

4. HETEROGENEOUS NUCLEATION INTENSITY

In order to determine and validate the heterogeneous nucleation rate, 12 experimental tests were performed for the N1 motive nozzle geometry. For the registered values of the critical mass flow rate a series of numerical simulations were performed (for DEM with the superposition of homogeneous and heterogeneous nucleation), based on which the values of φ were determined for each test point.

The values of φ proved to be dependent on the phase transition pressure (Figure 2), similar to the data presented in the literature, e.g. Gerum et al. (1979), Kolev (2007).



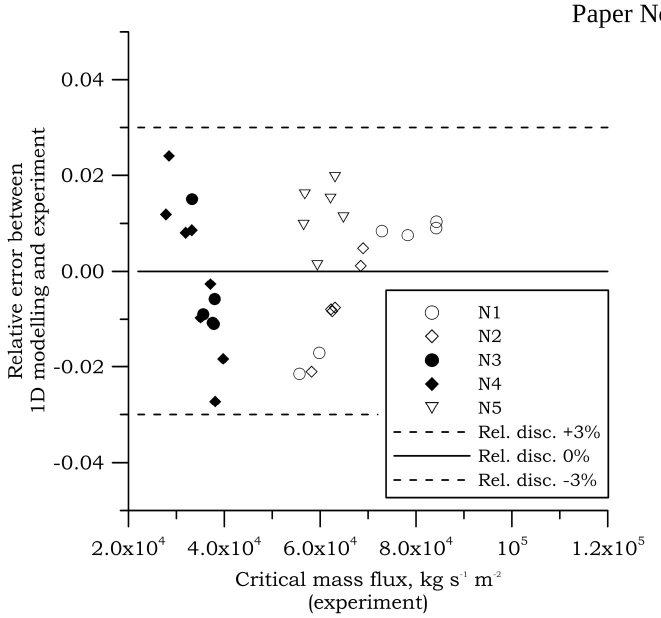


Figure 2. φ as a function of the metastable flashing pressure, averaged over the non-equilibrium section of the N1 nozzle flowpath (on the left), and relative error between the simulated and measured values of the critical mass flux (expressed per square meter of the throat cross-section area) for different geometries of the motive nozzle (on the right). The filled symbols represent condensation conditions, and the hollow symbols represent evaporation conditions.

After the approximation function for φ was implemented in the DEM model, 31 additional validation measurements were collected for 5 different geometry variants of the motive nozzle presented in Table 1 for the following test conditions:

- pressure of equilibrium phase change inception for isentropic expansion: from 6.230×10^6 Pa to 7.362×10^6 Pa,
- the critical mass flux: from 27.83×10^3 kg s^{-1} m^{-2} to 84.26×10^3 kg s^{-1} m^{-2}.

Based on the comparison between the experiments and the results of the numerical simulations (Figure 2) the authors considered the developed approach to be capable of sufficiently accurate prediction of the critical mass flux for the conically shaped converging-diverging R744 nozzles with sufficiently smooth wall surfaces (processed by finish grinding or lapping) for the examined ranges of the operating conditions. Therefore, further numerical analysis of the flow profiles could be performed.

5. EFFECTS OF NUCLEATION REGIME

The adapted model was utilized for the N1 geometry, for the motive nozzle inlet conditions typical for the gas cooler outlet in an R744 heat pump, namely 90 bar and 30 °C. This located the pressure of equilibrium phase change inception for isentropic expansion at 6.362×10^6 Pa. The simulated values of selected nozzle parameters for three possible phase transition regimes were collected in Table 2.

Table 2. Selected nozzle parameters for the N1 geometry for inlet conditions at 90 bar and 30 °C.

Phase transition regime	Critical mass flux	Expansion ratio	Isentropic efficiency
HEM	60.62×10^3 kg s^{-1} m^{-2}	1.83	93.6%
DEM (hom. & het. nucleation)	63.00×10^3 kg s^{-1} m^{-2}	1.98	89.8%
DEM (hom. nucleation)	72.88×10^3 kg s^{-1} m^{-2}	3.77	63.1%

Compared to the homogeneous and heterogeneous nucleation DEM, the critical mass flux computed according to the HEM was slightly (by 3.8%) underestimated, while for the homogeneous nucleation DEM was noticeably (by 15.7%) overvalued. The consequences of differences in the mass capacity were clearly visible in the decompression profiles for pressure and velocity (Figure 3) as well as in the values of the overall indicators like expansion ratio and isentropic efficiency (Table 2).

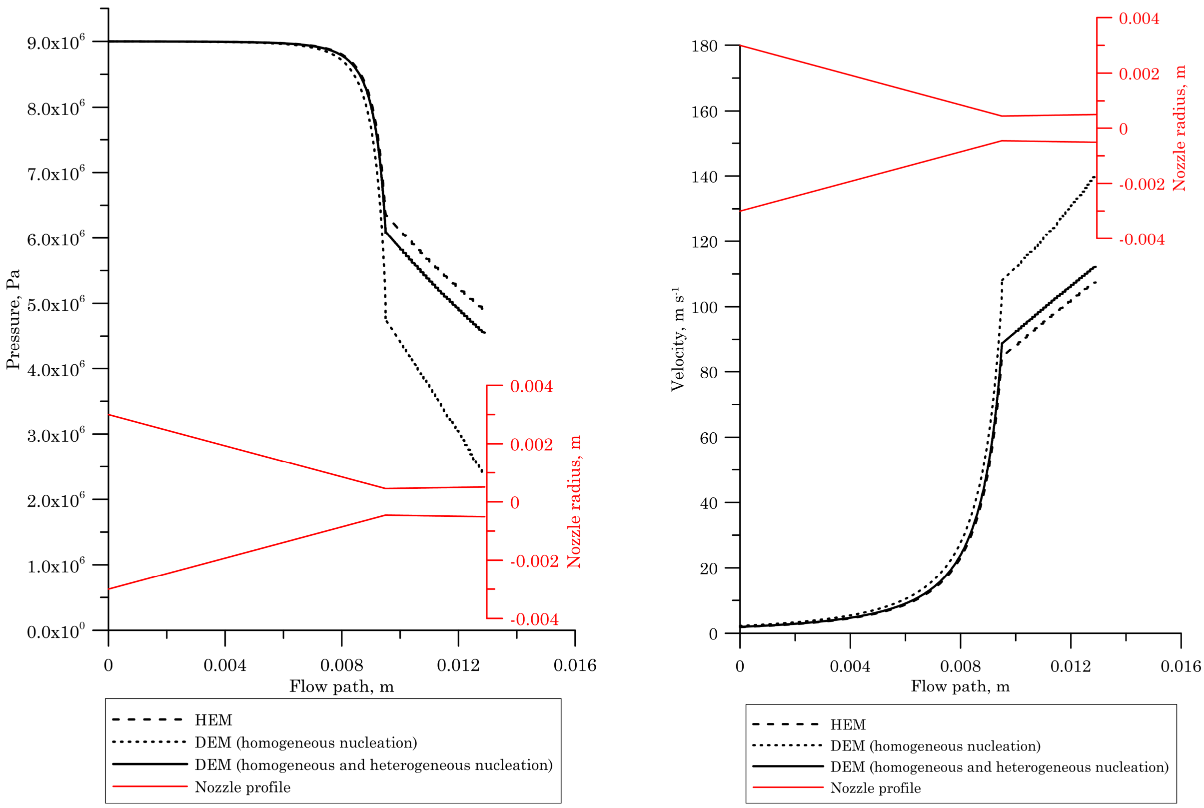


Figure 3. Simulated profiles of pressure (on the left) and velocity (on the right) for the N1 geometry for inlet conditions at 90 bar and 30 °C.

The analysis of the results suggests a possible trade off during the design process. In order to maximize the isentropic efficiency of the nozzle the overall nucleation rate should be intensified while for the maximization of the nozzle mass capacity the nucleation process should be inhibited. These can be adjusted mainly by augmentation/deterioration of the heterogeneous nucleation process (e.g. by coating the nozzle walls by thin layers of substances which chemical composition and surface structure could promote/prohibit formation of the critically sized clusters) since the homogeneous nucleation is determined solely by fluid properties and actual superheat/subcooling.

The simulated values of parameters expressing intensity of the phase transition processes for three possible regimes were collected in Table 3.

Table 3. Selected parameters of the expansion processes for the N1 geometry for inlet conditions at 90 bar and 30 °C.

Phase transition regime	**Metastable section length**	**Metastable section end quality**	**Metastable section pressure drop**	**Nozzle outlet quality**
HEM	0 m	0%	0 Pa	19.0%
DEM (hom. & het. nucleation)	30×10^{-6} m	5.1%	0.245×10^{6} Pa	22.0%
DEM (hom. nucleation)	160×10^{-6} m	20.5%	1.530×10^{6} Pa	36.7%

The simulated profiles of the equilibrium and actual gas fraction for three possible phase transition regimes were presented in Figure 4.

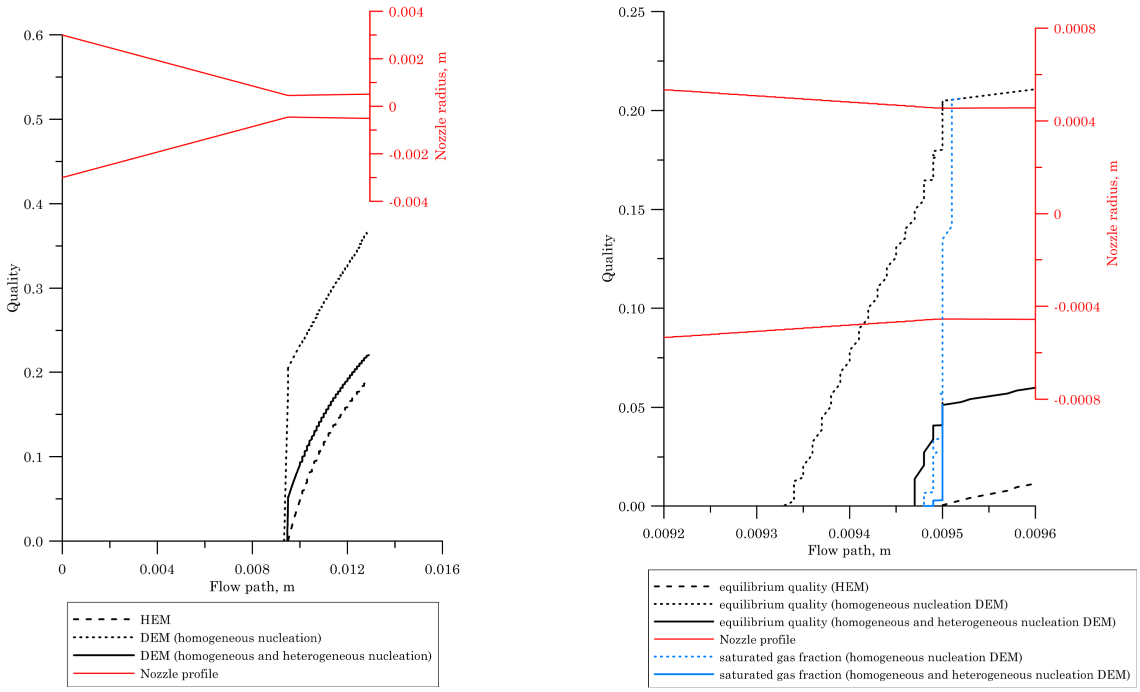


Figure 4. Simulated profiles of equilibrium quality (on the left) and magnifications of the saturated gas fraction profiles over the non-equilibrium sections (on the right) for the N1 geometry for inlet conditions at 90 bar and 30 °C.

The values of the equilibrium quality at the nozzle exit corresponded to the values of the overall expansion ratio and were highest for the homogeneous nucleation DEM. Similarly, as a consequence of a limited nucleation rate, the non-equilibrium section also proved to be longest and pressure drop highest for the same phase transition regime. It should be noted that, unlike for capillary tubes or orifices, the relative lengths of the metastable section (e.g. referenced to the length of the converging part) are extremely short and were equal to 0.32% for the homogeneous and heterogeneous nucleation DEM and 1.68% for the homogeneous nucleation DEM.

6. CONCLUSIONS

The metastability effects in the phase transition processes for transcritical R744 converging-diverging nozzles were investigated in this study. The simulation tool for the numerical analysis of the nozzle utilized the Delayed Equilibrium Model with a superposition of homogeneous and heterogeneous nucleation. The HEM approach vs. homogeneous nucleation DEM were considered the boundary cases for possible phase transition regimes.

Based on the results of the experimental tests for conical geometry, the authors validated the developed correlation equation for the nucleation work reduction factor for a typical range of operating conditions. The absolute values of the relative errors between the simulation and the experimental results for the critical mass flux were acceptably low and did not exceed 3%.

Moreover, the results suggested that purely homogeneous nucleation in the R744 supersonic nozzle may not be a realistic approach for typical cases and may lead to significant deviations from the real cases. On the other hand, the HEM approach may cause computational difficulties with numerical integration (especially in iterative algorithms) due to the discontinuity in the sonic speed, calculated according to the definition developed for the single-phase cases.

ACKNOWLEDGEMENTS

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NOMENCLATURE

Variables

A	throat diameter (m)
B	outlet diameter (m)
C	divergence half-angle (°)
φ	nucleation work reduction factor (-)

Abbreviations

DEM	Delayed Equilibrium Model
HEM	Homogeneous Equilibrium Model
HRM	Homogeneous Relaxation Model

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