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Parametric study of subsonic convergent nozzle expansion for cryogenic CO_2 applications

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Abstract

Cryogenic carbon dioxide (CO_2) capture relies on phase transitions, such as condensation or desublimation, induced by temperature reduction, enabling high-purity separation without chemical solvents. However, achieving the low temperatures required for CO_2 desublimation is energy-intensive and typically requires complex equipment. Subsonic convergent nozzles provide a mechanically simple alternative for direct-expansion cooling, yet their thermodynamic performance and operating limits remain poorly characterised, particularly in the context of cryogenic CO_2 processes. This study presents a parametric thermodynamic analysis of subsonic convergent nozzle expansion using a one-dimensional real-gas model constrained to strictly subsonic operation. A fixed-geometry nozzle based on a Witoszynski profile is considered to minimise internal losses, thereby promoting higher isentropic efficiency. The influence of inlet pressure, inlet temperature, pressure ratio, and isentropic efficiency on downstream properties, including temperature drop, mass flow rate, exit velocity, and exit Mach number, is systematically investigated. The results demonstrate that the pressure ratio is the dominant parameter governing cooling performance, with temperature drops reaching up to 35 K as the exit Mach number approaches unity. This condition defines the maximum attainable cooling under subsonic operation. Variations in inlet pressure have a limited effect on temperature reduction but significantly influence mass flow rate, while higher inlet temperatures lead to larger temperature drops. Variations in isentropic efficiency, reflecting different levels of internal losses, strongly affect both cooling intensity and the critical pressure ratio. Within the framework of cryogenic CO_2 processes, the analysis defines the achievable cooling range and identifies operating conditions under which subsonic expansion becomes compatible with CO_2 desublimation, providing a structured thermodynamic characterisation of subsonic nozzle performance and its intrinsic limitations.

Keywords

CO2 Capture; Desublimation; Direct Expansion Cooling; Subsonic Nozzle; Thermodynamic Analysis.

1. Introduction

Cooling processes play a critical role in industrial systems involving gas compression, transport, and processing [1]. Achieving efficient temperature reduction remains a key challenge, particularly due to the significant energy consumption associated with cooling technologies [2].

Expansion-based cooling provides a direct thermodynamic mechanism for temperature reduction, in which the acceleration of a compressible flow leads to a decrease in static pressure and temperature. This behaviour results from the conversion of internal energy into kinetic energy along the flow [3-4].

Nozzles are among the simplest devices capable of producing such expansions through the controlled variation of cross-sectional area [3,5]. In compressible flows, this leads to a reduction of static pressure and temperature under appropriate thermodynamic conditions [3-4].

Compared with conventional throttling processes, nozzle-based expansion can produce stronger temperature reductions due to its closer approximation to isentropic behaviour [6-8]. As a result, nozzle expansion has been widely investigated in applications involving rapid gas acceleration and thermal management [5,9].

Despite their simplicity, the majority of studies on nozzle-based expansion have focused on supersonic regimes, particularly in applications involving condensation, phase separation, and gas processing technologies [10-12]. In these systems, strong expansion effects enable the development of metastable conditions, leading to nucleation and phase transition phenomena [13-15].

In contrast, subsonic convergent nozzles are typically associated with more moderate temperature reductions and are often integrated within broader thermal management systems rather than used as standalone cooling devices [5,9]. However, despite extensive research on nozzle expansion in propulsion and compressible flow applications, the thermodynamic performance and operating limits of subsonic convergent nozzles for direct-expansion cooling remain insufficiently characterised, particularly in the context of cryogenic CO_2 capture. This gap is especially relevant for applications requiring sufficiently low temperatures to enable phase-change mechanisms such as condensation or desublimation. This work addresses that gap through a parametric thermodynamic analysis of subsonic convergent nozzle expansion, focusing on the influence of pressure ratio, inlet temperature, inlet pressure, and isentropic efficiency on the achievable cooling performance.

The main contribution of this work is the systematic thermodynamic characterisation of subsonic convergent nozzle expansion and the identification of operating conditions that are compatible with CO_2 desublimation under strictly subsonic constraints.

2. Methodology

2.1. Nozzle geometry

The expansion process analysed in this study is carried out using a convergent nozzle operating under subsonic conditions, with a fixed geometry throughout the analysis. The nozzle profile is based on a Witoszynski-type design, ensuring a smooth and continuous variation of the cross-sectional area along the flow direction.

The Witoszynski-type profile promotes a gradual acceleration of the flow, reducing adverse pressure gradients and minimising internal losses during expansion. Compared to simpler geometries such as conical nozzles, this results in improved isentropic efficiency. In particular, the smoother area variation contributes to higher isentropic efficiency by limiting flow separation and dissipative effects, which is critical for maximising the cooling performance under subsonic conditions.

Using a fixed geometry is a deliberate modelling choice. Rather than optimising the nozzle shape for specific operating conditions, the present study aims to isolate the influence of thermodynamic parameters on the expansion process. By maintaining a constant geometry, the influence of operating conditions on cooling performance can be assessed separately.

The nozzle consists of an inlet section followed by a converging region that progressively accelerates the flow towards the outlet. The geometry is defined to ensure that the flow remains entirely within the subsonic regime, with the Mach number approaching but not exceeding unity at the nozzle exit. This constraint reflects the operating limits of convergent nozzles and is consistent with the scope of the present study. The mass flow rate associated with this reference condition is not treated as a variable, as it is used only as a scaling parameter. The nozzle geometry is defined based on a reference design point, resulting in fixed inlet and outlet cross-sectional areas used throughout the analysis.

2.2. Thermodynamic model

The expansion process is analysed using a one-dimensional steady-flow thermodynamic model. The flow is assumed to be compressible and adiabatic, with no shaft work.

The working fluid is modelled as a dry flue gas mixture composed of 80% N_2, 5% O_2, and 15% CO_2 on a molar basis, ensuring that the thermodynamic analysis remains representative of CO_2-containing process streams relevant to carbon capture applications. Real-gas behaviour is considered, allowing thermodynamic properties to vary as a function of pressure and temperature along the expansion. This is particularly relevant for cooling processes, where significant variations in thermodynamic properties occur during expansion, especially near phase-change conditions.

To account for irreversibilities, the model incorporates a nozzle isentropic efficiency parameter, which represents the deviation from ideal isentropic expansion. This parameter is treated as a variable in the parametric analysis to evaluate its influence on both flow acceleration and temperature reduction. For the operating-map analysis, the CO_2 sublimation condition is evaluated based on its partial pressure, which is determined from the adopted gas composition. The CO_2 partial pressure is determined from its molar fraction in the mixture and the total pressure.

The present analysis focuses exclusively on CO_2 desublimation, while condensation phenomena are not considered. This thermodynamic criterion is later used to construct the operating map and identify regions compatible with CO_2 desublimation under strictly subsonic constraints.

2.3. Governing equations

The thermodynamic evolution of the expanding flow is described through the continuity, energy conservation, irreversibility, and Mach-number relations governing acceleration, cooling, and the subsonic operating limit.

For one-dimensional steady flow, the mass flow rate is defined by:

$$\dot{m} = \rho A V, \qquad (1)$$

where $\dot{m}$ is the mass flow rate, ρ is the gas density, A is the cross-sectional area, and V is the flow velocity. In the present model, this relation is used to ensure mass conservation along the nozzle, i.e. the same mass flow rate must be satisfied at every cross section. Therefore, as the cross-sectional area decreases, the flow velocity must increase, together with the corresponding adjustment in density under compressible conditions.

The conservation of energy for an adiabatic flow without shaft work is given by:

$$h_0 = h + \frac{V^2}{2}, \qquad (2)$$

where h_0 is the stagnation enthalpy and h the static enthalpy. As a direct consequence of the flow acceleration imposed by the convergent geometry, part of the static enthalpy is converted into kinetic energy. This thermodynamic relationship explains the reduction in static temperature observed during expansion. Between inlet and outlet states, this balance represents the ideal energy conversion mechanism, while deviations from this behaviour due to irreversibilities are subsequently accounted for through the nozzle isentropic efficiency.

The isentropic efficiency of the nozzle is defined as:

$$\eta = \frac{h_1 - h_2}{h_1 - h_{2s}}, \qquad (3)$$

where h_1 is the inlet enthalpy, h_2 the real outlet enthalpy, and h_{2s} the outlet enthalpy corresponding to an ideal isentropic expansion.

The local Mach number is given by:

$$M = \frac{V}{a}, \qquad (4)$$

where a is the local speed of sound. As previously noted, the analysis is constrained such that $M < 1$ throughout the nozzle, thereby ensuring subsonic operation.

2.4. Parametric analysis

A parametric study is conducted to evaluate the influence of operating conditions on the expansion process and the resulting cooling performance. The parametric analysis is performed around a reference operating condition (200 kPa, 213.5 K), with inlet pressure and temperature varied over representative ranges relevant to cryogenic CO_2 processes.

The analysis considers the influence of pressure ratio, inlet temperature, inlet pressure, and isentropic efficiency. These parameters are varied independently while keeping the nozzle geometry fixed. For each set of conditions, the thermodynamic state of the flow is evaluated, enabling the determination of key quantities such as temperature drop, exit velocity, mass flow rate, and Mach number.

Particular attention is given to the influence of the pressure ratio, as it governs the intensity of the expansion process and the approach to the sonic limit at the nozzle outlet. This limit defines the maximum achievable expansion in a purely convergent nozzle operating under subsonic conditions and is central to the analysis presented in this study. In practice, the subsonic operating threshold is identified based on an outlet Mach number close to unity.

3. Results and discussion

The thermodynamic model described in the previous section is applied to evaluate the cooling performance of subsonic expansion in a convergent nozzle with fixed geometry.

3.1. Influence of pressure ratio

The pressure ratio between inlet and outlet conditions is the primary parameter governing the intensity of the expansion process and, consequently, the achievable cooling.

Figure 1 illustrates the evolution of the outlet Mach number and the temperature drop as functions of the pressure ratio. For pressure ratios close to unity, the expansion is weak, resulting in negligible temperature reduction and limited flow acceleration. As the pressure ratio increases, the conversion of static enthalpy into kinetic energy becomes more pronounced, leading to increased flow velocity and reduced static temperature.

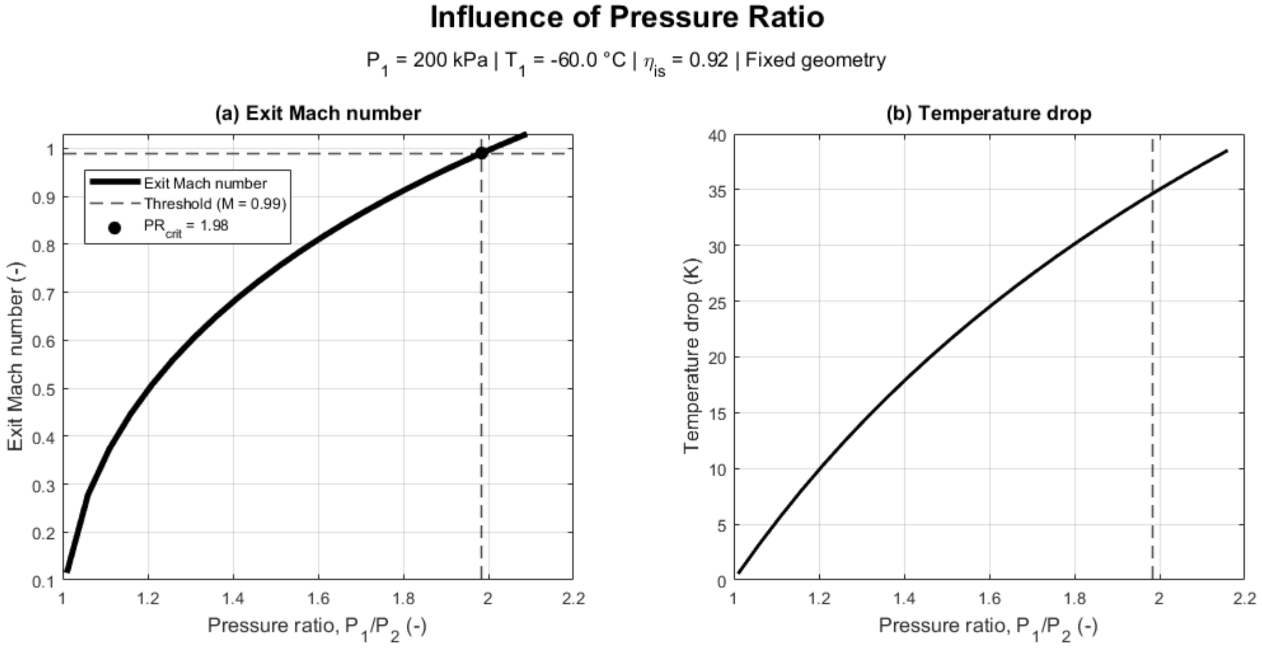

Figure. 1. *Influence of pressure ratio on subsonic nozzle expansion: (a) exit Mach number vs pressure ratio; (b) temperature drop vs pressure ratio.*

Figure 1(a) shows that the outlet Mach number increases monotonically with pressure ratio and approaches the sonic condition (M = 1). This behaviour defines the subsonic operating limit of the convergent nozzle, beyond which further expansion cannot be sustained.

Figure 1(b) indicates that the temperature drop increases with pressure ratio, reaching approximately 35 K near the subsonic limit. The increase in temperature drop is non-linear, with a progressively lower rate of increase as the flow approaches the sonic condition. This indicates a diminishing return in cooling performance as the expansion limit is approached. The critical pressure ratio associated with the subsonic limit is found to be 1.98 for the reference conditions. This behaviour establishes a fundamental thermodynamic constraint: the maximum attainable cooling in subsonic expansion is intrinsically limited by the approach to the sonic condition, regardless of further increases in the pressure ratio. This physical limit defines the maximum cooling potential of subsonic convergent expansion and provides the basis for assessing whether the remaining cooling capacity can support CO_2 desublimation under suitable inlet conditions.

3.2. Influence of inlet conditions

The inlet conditions influence the expansion process through distinct physical mechanisms. In particular, the inlet temperature affects the thermodynamic potential for cooling, whereas the inlet pressure plays a secondary role when the pressure ratio is fixed.

Figure 2 presents the influence of inlet temperature and inlet pressure on the temperature drop under fixed pressure ratio conditions.

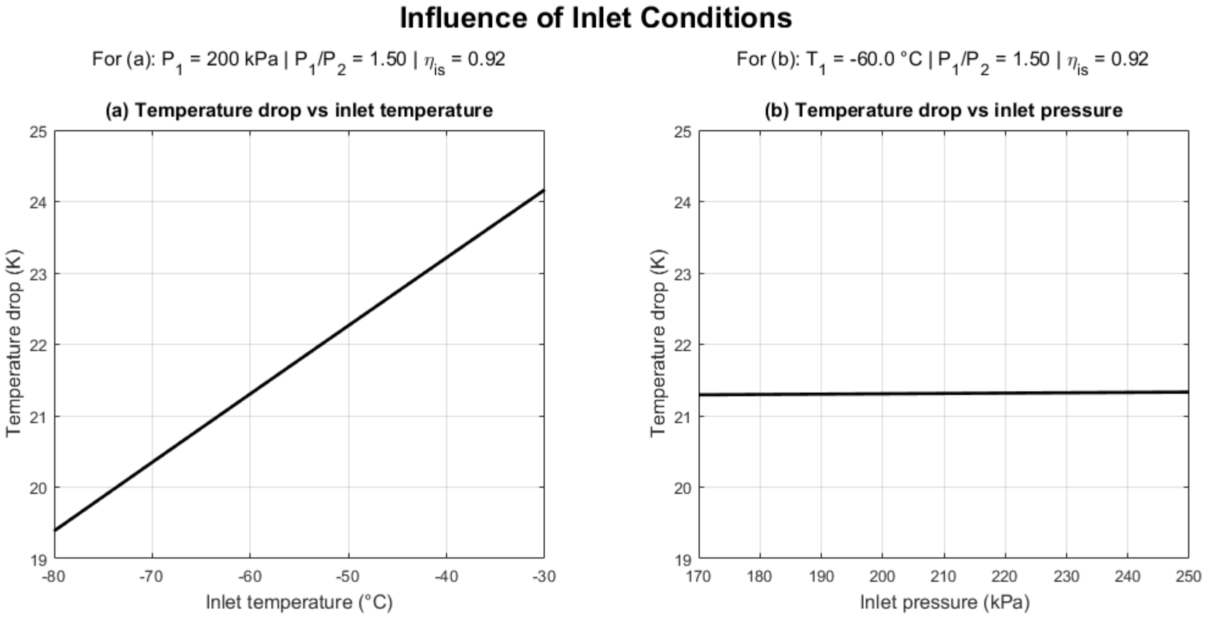

Figure. 2. *Influence of inlet conditions on subsonic nozzle expansion at fixed pressure ratio: (a) temperature drop vs inlet temperature; (b) temperature drop vs inlet pressure.*

As shown in Figure 2(a), the temperature drop increases with increasing inlet temperature. For higher inlet temperatures, the available enthalpy difference during expansion is greater, leading to a larger conversion of static enthalpy into kinetic energy. Consequently, a greater temperature reduction is achieved.

In contrast, Figure 2(b) indicates that variations in inlet pressure at fixed pressure ratio have a negligible effect on the resulting temperature drop. The temperature reduction remains essentially constant across the analysed pressure range, indicating that the cooling performance is primarily governed by the pressure ratio rather than the absolute pressure level.

In summary, for a given nozzle geometry and pressure ratio, the inlet temperature is the dominant parameter controlling the magnitude of cooling, while the inlet pressure has very little influence on the thermodynamic outcome of the expansion.

3.3. Influence of isentropic efficiency

The isentropic efficiency represents the degree to which internal losses affect the expansion process and, consequently, the achievable cooling performance.

Figure 3 presents the variation of the temperature drop as a function of the isentropic efficiency, with all other parameters fixed. As the efficiency increases, the temperature drop increases approximately linearly, reflecting a more effective conversion of static enthalpy into kinetic energy.

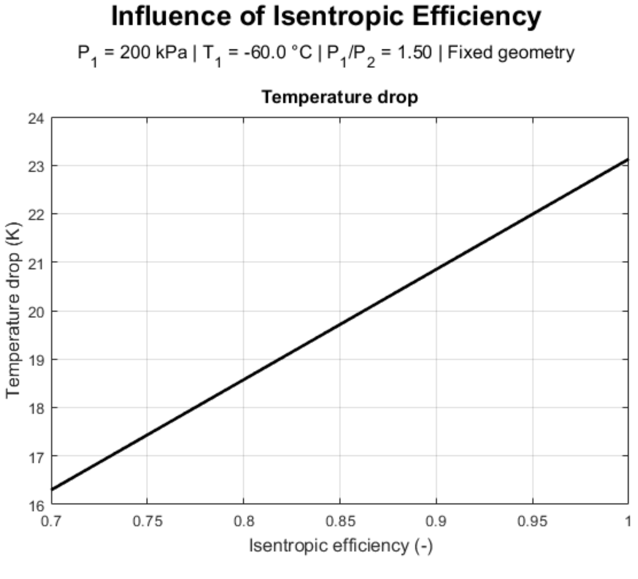

Figure. 3. *Influence of isentropic efficiency on subsonic nozzle expansion: temperature drop vs isentropic efficiency.*

For lower efficiency values, a larger fraction of the available enthalpy is dissipated by irreversibilities, resulting in reduced flow acceleration and lower temperature reduction. As efficiency approaches unity, these losses are minimised, leading to the maximum attainable cooling for the given pressure ratio and inlet conditions.

Overall, the results indicate that isentropic efficiency significantly affects cooling performance, although its effect remains secondary compared to the influence of the pressure ratio.

3.4. Operating map and desublimation conditions

Figure 4 presents the operating map of the fixed-geometry subsonic nozzle, highlighting the different regimes as a function of inlet temperature and pressure ratio. Building on the previously identified cooling limits and parametric sensitivities, it defines the practical thermodynamic window for desublimation-compatible subsonic operation.

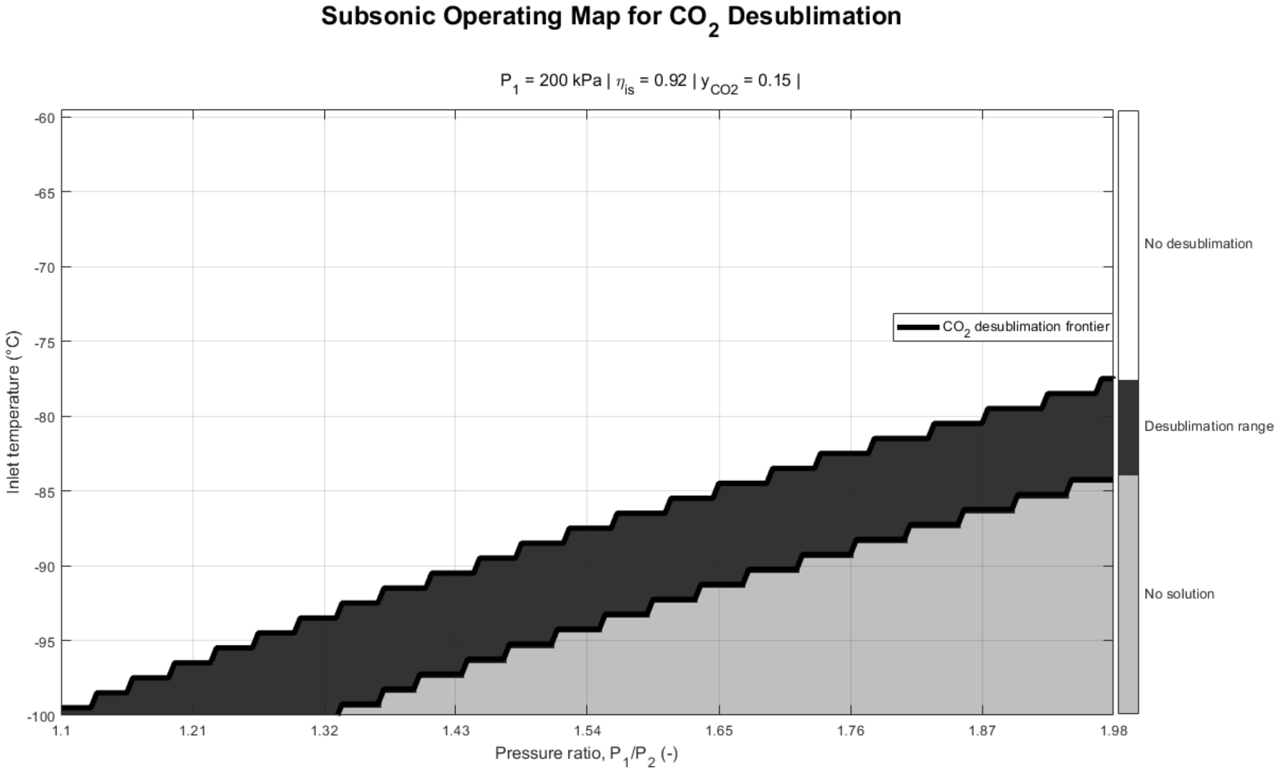

Figure. 4. *Operating map of the fixed-geometry subsonic nozzle: classification of operating regimes as a function of inlet temperature and pressure ratio.*

This map reveals three distinct operating regimes, defined by the feasibility of subsonic expansion and thermodynamic compatibility with CO_2 desublimation: a) a *no-solution* regime, in which the required expansion exceeds the physical limit imposed by the sonic condition; b) a subsonic *no-desublimation* regime, in which the flow remains subsonic but the outlet state lies outside the desublimation region; and c) a *desublimation range* regime, in which the flow remains subsonic and the outlet state falls within the desublimation range.

The transition between the three regimes is governed by the combined effect of inlet temperature and pressure ratio. Lower inlet temperatures and higher pressure ratios favour the onset of desublimation-compatible conditions, as they promote larger temperature reductions during expansion.

The desublimation frontier shown in Figure 4 represents the thermodynamic boundary at which the outlet state reaches the CO_2 sublimation condition based on its partial pressure in the gas mixture. This boundary therefore defines the limit of thermodynamic compatibility with desublimation.

The desublimation range identified in the map represents thermodynamic feasibility only. The actual formation of solid CO_2 particles depends on additional factors, including nucleation and growth kinetics, which are not considered in the present analysis. The present analysis is based on a one-dimensional thermodynamic model and does not account for multi-dimensional flow effects or detailed phase-change kinetics.

Overall, the results show that subsonic nozzle expansion, although inherently limited by the sonic condition, can still reach thermodynamic states compatible with CO_2 desublimation under specific operating conditions.

4. Conclusions

This study presents a parametric thermodynamic analysis of subsonic convergent nozzle expansion under conditions relevant to cryogenic CO_2 applications, using a fixed-geometry configuration and a one-dimensional real-gas model.

The results show that the pressure ratio is the dominant parameter governing cooling performance. As the pressure ratio increases, the temperature drop increases significantly, but this behaviour is inherently limited by the subsonic operating constraint, as the outlet Mach number approaches unity. This defines a fundamental thermodynamic ceiling for subsonic expansion.

Inlet conditions affect the expansion asymmetrically. The inlet temperature directly controls the magnitude of the achievable cooling, whereas the inlet pressure has a negligible impact when the pressure ratio is fixed. Isentropic efficiency also plays an important role, as higher values correspond to lower internal losses and, consequently, to larger temperature drops.

The operating map provides a structured interpretation of nozzle behaviour, identifying three distinct regimes: no subsonic solution, subsonic operation without desublimation, and subsonic operation within the desublimation range. This classification shows that, despite the intrinsic limitations of subsonic expansion, thermodynamic conditions compatible with CO_2 desublimation can still be achieved within a well-defined operating window.

Overall, the results show that subsonic convergent nozzles, although physically constrained, constitute a viable solution for simplified cooling and pre-conditioning stages in cryogenic CO_2 capture systems.

Nomenclature

A	nozzle cross-sectional area, m²
a	speed of sound, m/s
h	specific enthalpy, J/kg
h_0	stagnation enthalpy, J/kg
h_1	inlet specific enthalpy, J/kg
h_2	outlet specific enthalpy, J/kg
h_{2s}	isentropic outlet specific enthalpy, J/kg
M	Mach number, -
$\dot{m}$	mass flow rate, kg/s
P	pressure, kPa
T	temperature, K
V	flow velocity, m/s

Greek symbols

η	isentropic efficiency, -
ρ	density, kg/m³

Subscripts

1	inlet condition
2	outlet condition
s	isentropic condition

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