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NiceProp: An interactive Python-based educational tool for non-ideal compressible fluid dynamics

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ABSTRACT

Non-ideal compressible flows exhibit physical behaviors that are quantitatively and qualitatively different than those of a perfect or ideal gas. As such, the classical gas dynamic relationships that can be found on fluid-mechanics textbooks cannot be directly applied to characterize this type of flows. NiceProp is a tool for interactively learning the fundamentals of non-ideal compressible fluid dynamics and the design implications for fluid machinery components. The software is written in Python and features a highly modular structure to ease code readability and to facilitate its further development. The target audience of the software is represented by students, researchers and industry professionals interested to get started or deepen the comprehension of non-ideal compressible flow phenomena.

Code metadata

Current code version	v1.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-21-00170
Legal Code License	GNU General Public License, version 3 (GPLv3)
Code versioning system used	Git
Software code languages, tools, and services used	Python 3
Compilation requirements, operating environments & dependencies	REFPROP license to use the REFPROP backend in CoolProp, https://github.com/usnistgov/REFPROP-cmake to build the REFPROP shared library in Unix-like OS
If available Link to developer documentation/manual	https://github.com/Propulsion-Power-TU-Delft/NiceProp
Support email for questions	a.giuffre@tudelft.nl

1. Motivation and significance

Non-ideal compressible fluid dynamics (NICFD) is the branch of fluid mechanics concerning non-reacting flows of fluids in non-ideal thermodynamic states. It therefore deals with dense vapor flows, two-phase vapor–liquid flows and compressible liquid flows [1]. In these flow regimes, compressibility effects induce a significant departure from the well-known gas dynamic behavior of dilute, constant-specific-heat gases, under both a quantitative and a qualitative point of view. In the following, fluid ideality refers to the thermodynamics of perfect gases, governed by the $Pv = RT$ and $c_v =$ const. equation of state, where P, T, v, R, c_v stand for pressure, temperature, specific volume, specific gas constant, and specific heat capacity at constant volume, respectively. On the opposite, for non-ideal compressible flows $Pv \neq RT$ and the classical gas dynamic relationships, e.g., $P_t/P = f(M, \gamma)$, where M and γ are the Mach number and the specific heat capacity ratio, do not hold anymore.

Engineering applications where non-ideal flows typically occur are fluid machinery and heat exchangers of organic Rankine cycle (ORC) turbogenerators and of supercritical CO_2 power systems [2–4]. Turbomachinery and heat exchangers of heat pumps [5,6] and refrigeration systems [7] are also components whose performance is affected by the occurrence of non-ideal flow effects. Other engineering applications operating with non-ideal flows are fluid machinery for the oil & gas industry [8], fuel injectors for high-pressure combustors [9], rocket engines [10], compressors and turbines for cryogenic plants [11]. In NICFD,

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depending on the fluid thermodynamic state, unconventional gas dynamic phenomena may arise, i.e. the speed of sound can increase across isentropic expansions and the Mach number can decrease along expansion processes. A summary of unconventional gas dynamic phenomena associated to NICFD is described in [12,13]. Peculiar fluid dynamic regimes characterized by the physical inversion of shock waves and expansion fans [14] also belong to NICFD.

Gaining a thorough physical understanding of non-ideal flow effects and their impact on the design of fluid machinery components is paramount to develop efficient flow devices. Many studies have been conducted so far to investigate non-ideal compressible effects in paradigmatic flow processes or in actual internal flow devices by means of numerical models [15,16] and experimental techniques [17,18] and substantial knowledge has already been developed and established. However, for anyone approaching NICFD, the conceptualization of such knowledge remains a cumbersome and lengthy process. One of the reason thereof is the lack of use of a common terminology within the NICFD community, albeit recent efforts to provide a unified theoretical framework [19]. Moreover, the learning process is somewhat hampered by the absence of open-source educational tools, contrarily to classical gas dynamics where online calculators for ideal flows are widely available [20]. These calculators can be very helpful to assimilate basic concepts of complex flows and related design aspects. All these limitations arguably make the learning curve for the non-experts approaching NICFD very steep.

NicePropp is a Python-based educational tool to interactively learn non-ideal compressible fluid-dynamics specifically built for ease of use and further development. The current version of the program addresses dilute and dense vapor flows for arbitrary fluids and their effect on the design of stationary fluid machinery devices, namely nozzles of turbines and diffusers of compressors. The target audience of the tool is not only scientists and industry professionals new to NICFD, but also more experienced practitioners who wish to gain a more solid and practical understanding of this fascinating field of science.

The structure of the paper is as follows. The theoretical foundations of NICFD are briefly summarized in Section 2. The software architecture is described in Section 3. The features of NiceProp are presented by examples of application in Section 4. The impact of this work and the concluding remarks are documented in Sections 5 and 6 .

2. Theoretical background

2.1. Dimensionless flow properties characterizing compressible dense vapors

The ideal gas equation of state reads

$$P = \rho RT \tag{1}$$

If Eq. (1) holds, then the compressibility factor $Z = P/(\rho RT)$ is unitary. Dense vapors, i.e. fluid states close to the critical point or close to the dew line, do not obey the ideal gas law, i.e. $Z < 1$. In this case, the isobaric and isochoric heat capacity, and their ratio $\gamma = c_p/c_v$ vary depending on the fluid state, thus hindering the use of the classic gas dynamic relationships.

Fluid dynamic processes occurring in the dense vapor region can be better examined resorting to secondary dimensionless state properties calculated through an equation of state model as function of, i.e., T, s or P, T. Isentropic flows of dense vapors can be described by the thermodynamic relation

$$P/\rho^{\gamma_{Pv}} = \text{const.}, \tag{2}$$

Table 1
Secondary thermodynamic properties relevant for the study of one dimensional dense vapor flows.

Definition	Ideal gas
$\gamma_{Pv} = -\frac{v}{P}\frac{c_p}{c_v}\left(\frac{\partial P}{\partial v}\right)_T$	γ
$\gamma_{PT} = \frac{1}{1-\frac{P}{c_p}\left(\frac{\partial v}{\partial T}\right)_P}$	γ
$\gamma_{Tv} = 1+\frac{v}{c_v}\left(\frac{\partial P}{\partial T}\right)_v$	γ
$\Gamma = 1+\frac{\rho}{c}\left(\frac{\partial c}{\partial \rho}\right)_s$	$\frac{\gamma+1}{2}$
$G = \frac{1}{\rho c_v}\left(\frac{\partial P}{\partial T}\right)_\rho = \gamma_{Pv}\gamma_{PT}$	γ^2

in analogy with the classic gas dynamic equation governing isentropic flows of ideal gases. If temperature and pressure are chosen as primary variables, the governing law of the isentropic process becomes

$$TP^{\frac{1-\gamma_{PT}}{\gamma_{PT}}} = \text{const.} \tag{3}$$

Alternatively, if temperature and density (or specific volume) are taken as primary variables, then the thermodynamic relation reads

$$Tv^{\gamma_{Tv}-1} = \text{const.} \tag{4}$$

γ_{Pv}, γ_{PT}, and γ_{Tv} are named generalized isentropic exponents [21,22] and their definitions are reported in Table 1. The product between γ_{Pv} and γ_{PT} is termed as Grüneisen parameter G. Its use in fluid dynamics theory is however quite limited. If the perfect gas law is valid, the three isentropic exponents reduce to the specific heat capacity ratio γ, and G to γ^2.

Differentiating Eq. (2) with respect to the specific volume leads to

$$\Gamma = \frac{1}{2}\left[\gamma_{Pv} + 1 - \frac{v}{\gamma_{Pv}}\left(\frac{\partial \gamma_{Pv}}{\partial v}\right)_s\right] \tag{5}$$

Γ is termed fundamental derivative of gas dynamics [23] and is related to the variation of the speed of sound with density over an isentropic process. If $\Gamma > 1$, the sound speed decreases along an isentropic compression and increases over an expansion. This thermodynamic condition is representative of fluids in the dilute gas state, characterized by small variations of thermodynamic properties, for which the approximations $\Gamma \simeq (\gamma_{Pv} + 1)/2$ and $\gamma_{Pv} \approx$ const. are valid. On the opposite, if $\Gamma < 1$, the speed of sound increases over compressions and decreases over expansions, leading to quantitative deviations with respect to the ideal gas behavior. Furthermore, it is theoretically predicted that the so-called Bethe-Zel'dovich-Thompson (BZT) fluids [24], i.e. fluids characterized by heavy and complex molecules, exhibit a thermodynamic region where $\Gamma < 0$. In this peculiar thermodynamic states, it is possible to observe non-classical gas dynamic phenomena, such as rarefaction shock waves and compression fans [14].

The gas dynamic characteristics of dense vapor flows are highly affected by the values assumed by the secondary state properties over the prescribed thermodynamic transformation. Among them, γ_{Pv} and Γ are better suited for the description of fluid dynamic processes. For instance, insights of dense vapor effects in flow devices, i.e. nozzles, diffusers, and more complex fluid machinery, can be inferred by using the generalized form of the one-dimensional isentropic relations, written as function of γ_{Pv} or Γ [4,13,19,25]. Such relationships strictly hold if γ_{Pv} or Γ

are constant along the thermodynamic process. However a first-order approximation of the actual flow behavior can be obtained by using the averaged value of γ_{Pv}, defined as

$$\overline{\gamma_{Pv}} = \frac{ln\left(\frac{P_1}{P_2}\right)}{ln\left(\frac{\rho_1}{\rho_2}\right)}, \tag{6}$$

where the subscripts 1 and 2 correspond to the initial and final states of the prescribed transformation. This approximation becomes increasingly inaccurate while approaching the fluid critical point, where the secondary state properties exhibit strongly non-linear, and eventually non-monotonic, behavior.

2.2. Interactively learning NICFD

According to the authors' experience, an effective process of learning NICFD should encompass (i) a conceptual understanding phase, in which the theoretical concepts previously described are internalized through simple visual representations, (ii) a practical understanding phase, which must provide insights about the impact of flow non-ideality on the design of actual internal flow devices. NicePro offers a seamless learning experience by integrating features that can interactively enable both types of understanding.

The current version of the program allows one to investigate the influence of dense vapor effects on the flow characteristics and design of stationary fluid machinery components, namely converging–diverging nozzles, conical and radial diffusers. To start with, isentropic expansion or compression processes can be graphically displayed on the contours of the secondary state properties reported in Table 1 on the reduced T-s or P-T thermodynamic diagram. This way, one can learn (i) whether the physical process of interest occurs in the dilute gas or dense vapor region, (ii) the expected magnitude of dense vapor effects by comparing the averaged values of, e.g., Z, γ_{Pv} or Γ with those of the ideal gas and (iii) the expected trends of flow quantities by resorting to the generalized isentropic relations. Then, practical design aspects can be studied using the features that provide the preliminary shape of the internal flow device of interest. By means of this capability, the user can examine (i) the variation of shape of the fluid machinery components designed to operate with arbitrary fluid molecules and in different thermodynamic conditions (ii) the actual trend of flow quantities in these devices. The theoretical and practical concepts learnt by analyzing such paradigmatic examples can be then applied to efficiently design more complex fluid machinery components, e.g. supersonic stators of ORC turbines.

2.3. Design of nozzles and diffusers operating with dense vapors

The purpose of NicePro is to provide a user-friendly framework to learn NICFD and to evaluate the impact of flow non-ideality prior to approaching the detailed design of an internal flow device. Therefore, NicePro should not be intended as a tool to achieve the optimal design of fluid machinery components. With this idea in mind, the authors adopted a simplified approach for the preliminary design and analysis of flow devices, as described in the following. Nonetheless, the predictions obtained by NicePro show good agreement with those computed with more advanced numerical methods, as discussed in Section 4.4.

Isentropic flows in nozzles are calculated by combining the one-dimensional mass and energy balance equations, leading to

$$h_t = h(P, s) + \frac{\dot{m}^2}{2\rho^2(P, s)A^2}, \tag{7}$$

where A is the flow passage area. For a given inlet thermodynamic state, pressure ratio P_t/P or volumetric flow ratio ρ_t/ρ, and inlet flow velocity, the static pressure at inlet, throat, and outlet sections are first computed. Eq. (7) is then used to find the corresponding passage areas for a prescribed value of mass flow rate. The nozzle area distribution is obtained by means of the following law, valid for both the converging as well as the diverging part

$$R(x) = a + b\tanh(cx - d), \tag{8}$$

where $R(x)$ corresponds to the channel semi-width for a rectangular nozzle or the channel radius for a conical nozzle, and a, b, c, d are user-defined coefficients enabling the control of the geometry.

The calculation procedure for isentropic diffuser flows follows from the physical process occurring in an ideal compressor constituted by an impeller and a diffuser. For a given total-to-static pressure ratio of the compressor, flow velocity at the outlet of the diffuser, and a prescribed diffuser pressure recovery, the inlet and outlet diffuser passage areas are computed by solving the energy balance. Then, the treatment differs according to the diffuser configuration, i.e., radial or conical. The area distribution of a conical diffuser is determined by setting the value of the semi-aperture angle ϵ, once the inlet and outlet radii are computed. The thermodynamic flow properties at each section are finally calculated by numerically solving Eq. (7). On the contrary, two additional input quantities, H/R_{in} and α_{in}, are needed to compute the flow quantities in a radial diffuser, α_{in} being the flow direction at diffuser inlet. In this case, the flow governing equations read

$$\begin{aligned} \dot{m} &= \rho(P, s)V_m 2\pi RH \\ RV_t &= \text{const.} \\ h_t &= h(P, s) + \frac{V_t^2}{2} + \frac{V_m^2}{2} \end{aligned} \tag{9}$$

The inlet and outlet radii R_{in} and R_{out} are computed using the mass balance and assuming that $H_{in} = H_{out}$. For each intermediate radius, the system of equations is numerically solved to determine the unknowns P, V_t, V_m, and eventually all the remaining thermodynamic properties.

3. Software architecture

NicePro is written in native Python 3 using object-oriented programming. In order to compute the thermo-physical properties of arbitrary working fluids, the code is coupled to the open-source CoolProp software [26] by means of the low-level interface. The user can therefore decide to compute the fluid properties according to the built-in CoolProp models (PR, SRK, HEOS), or the models available in REFPROP [27] distributed by NIST.

The structure of the program is illustrated in Fig. 1. The main classes of NicePro are: `ThermodynamicModel`, `IsentropicFlowModel`, and `Plot`. The attributes of the class `ThermodynamicModel` are inherited by `IsentropicFlowModel` upon instantiation. The same applies to the `Plot` class with the attributes of `ThermodynamicModel` and `IsentropicFlowModel`. `ThermodynamicModel` contains the methods to calculate: (i) the dew and bubble lines; (ii) the thermodynamic states of the fluid within a user-defined region either in terms of pressure and temperature (`PTContour`), or temperature and entropy (`TsContour`); (iii) the non-ideal flow properties described in Section 2. The user-defined domain is discretized by means of a structured grid, in which the spacing along the two independent thermodynamic axes is determined by the variable `samples`. `IsentropicFlowModel` implements in `IdealProcess` the algorithm to compute the flow quantities along an

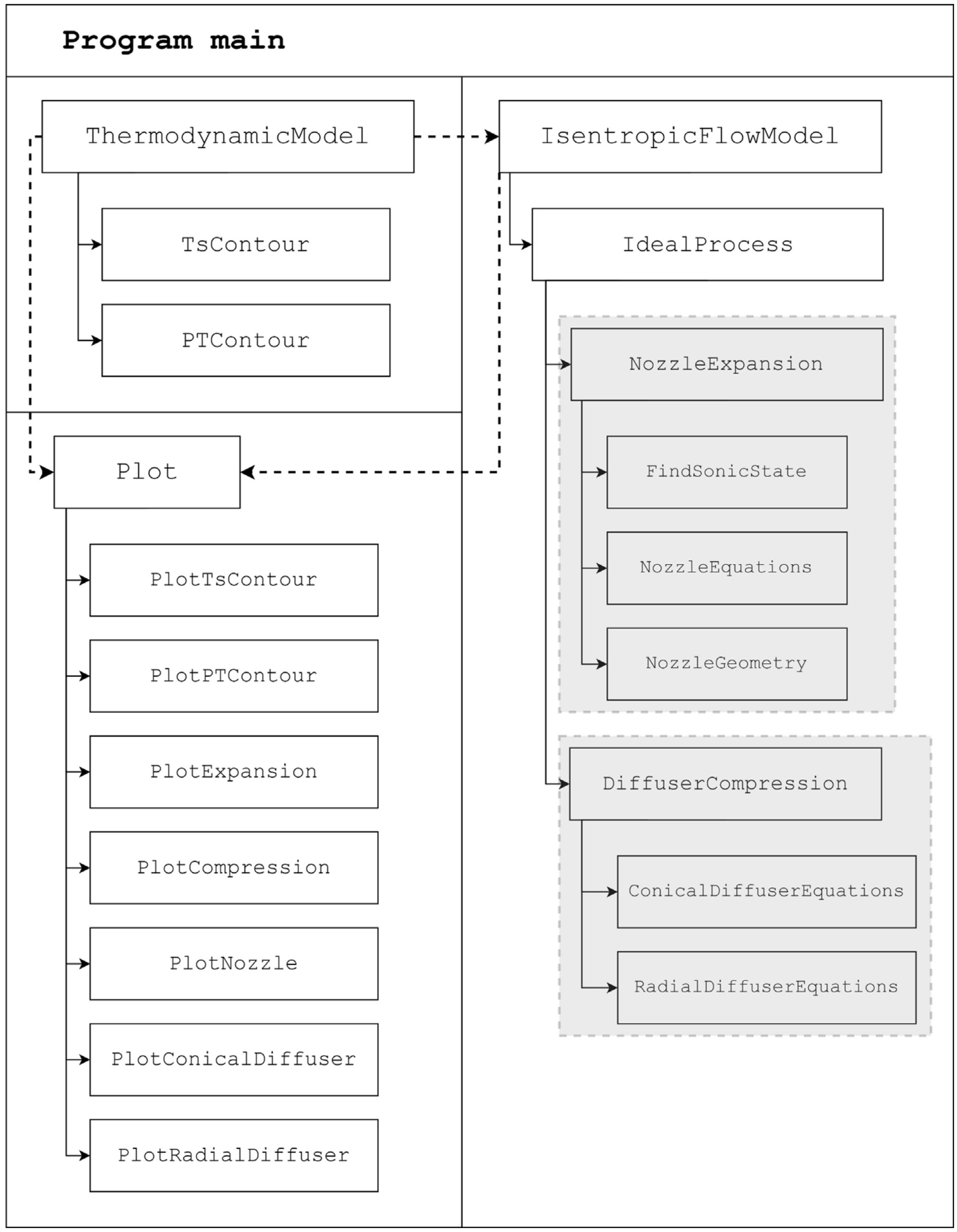


Fig. 1. NiceProp software architecture. The two main classes `ThermodynamicModel` and `IsentropicFlowModel` are instantiated in the program main. `IsentropicFlowModel` implements two sets of methods for the design of nozzle and diffuser, identified by the shaded regions.

isentropic expansion or an isentropic compression. The preliminary design procedures for converging–diverging nozzles, radial and conical diffusers, based on the solution of the conservation laws under the assumption of isentropic flow, are implemented in `NozzleExpansion`, and `DiffuserCompression`, respectively. The integral form of the governing equations is solved along a mean streamline, in which the number of computed states is determined by the number of `samples` selected in class `ThermodynamicModel`. The methods used to render and visualize the results are implemented in the class `Plot`.

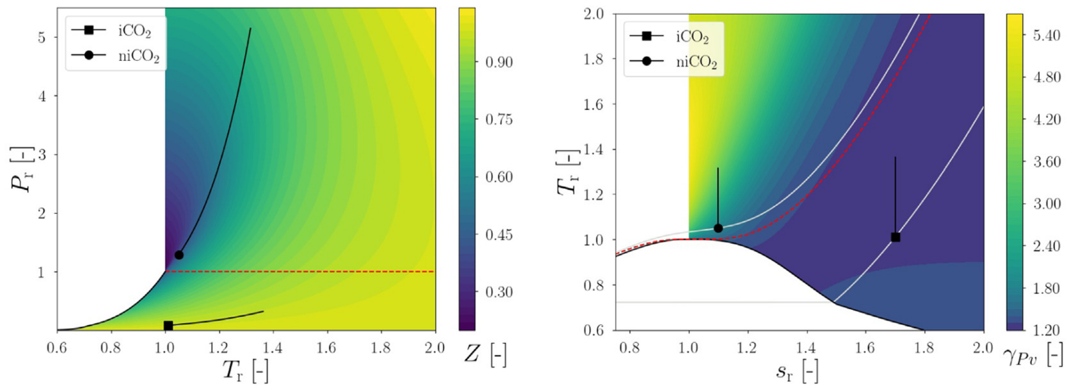
3.1. Input/output

The user-defined input required to run NiceProp is a configuration file written in standard text format and located in the input directory. The configuration file can be easily formatted by editing one of the examples released with the software. The available choices for each entry of the configuration file are clearly stated in the headers. An exemplary configuration file for NiceProp is reported in Appendix for convenience. Further information is available in the software documentation.

After a successful run, NiceProp stores all the results in a folder labeled with the name of the selected working fluid and located in the output directory. All the charts generated by NiceProp are saved both in *.jpeg* and *.tiff* format.

4. Illustrative examples

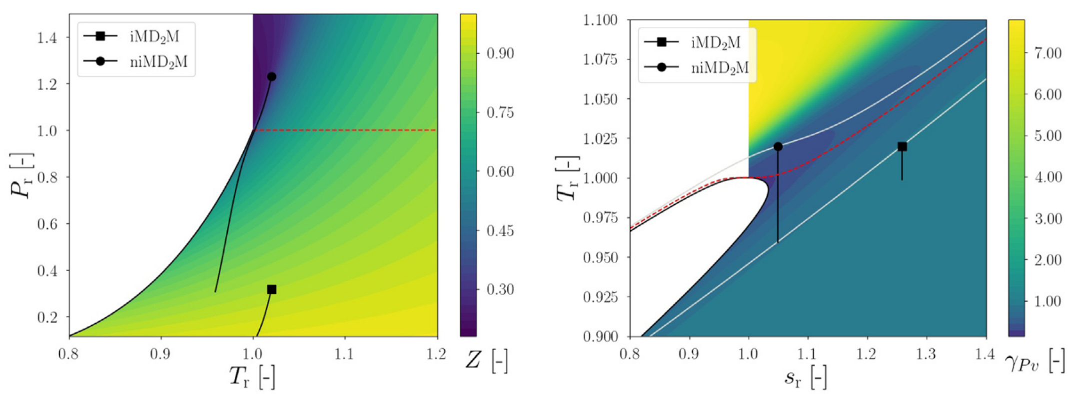
The capabilities of the software are illustrated by means of three examples: (1) the graphical representation of isentropic expansion and compression processes on the contours of Z and γ_{Pv} on the reduced T-s and P-T thermodynamic diagram; (2) the design of converging–diverging nozzles for siloxane MD_2M in the dilute and in the dense gas region; and (3) the design of radial diffusers for CO_2 in the vapor and in the supercritical region. The first example is meant for enabling conceptual understanding



(a) Compressibility factor in the $P_r - T_r$ thermodynamic plane

(b) Isentropic pressure-volume exponent in the $T_r - s_r$ thermodynamic plane

Fig. 2. Contours of non-ideal properties for CO_2. The saturation curve and the critical isobar are depicted by the solid black line and the dashed red line, respectively. The marked black lines identify two compression processes occurring in the dilute and dense gas region, see Table 2, for a pressure P_t/P ratio equal to 4. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



(a) Compressibility factor in the $P_r - T_r$ thermodynamic plane

(b) Isentropic pressure-volume exponent in the $T_r - s_r$ thermodynamic plane

Fig. 3. Contours of non-ideal properties for siloxane MD_2M. The saturation curve and the critical isobar are depicted by the solid black line and the dashed red line, respectively. The marked black lines identify two expansion processes occurring in the dilute and dense gas region, see Table 2, for a pressure ratio P_t/P equal to 4. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

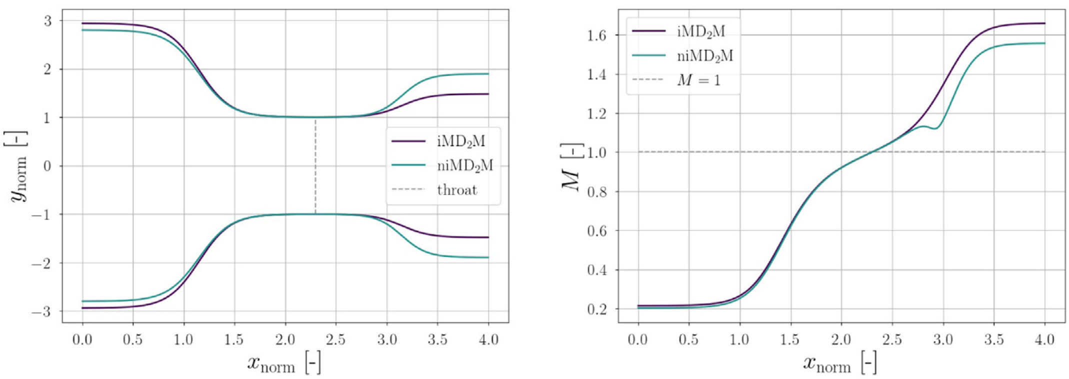
Table 2
Fluid properties and reduced inlet conditions selected for the illustrative examples.

Label	Fluid	P_r [-]	T_r [-]	$R\left[\frac{J}{kg \cdot K}\right]$	$\overline{Z}$ [-]	$\overline{\gamma_{Pv}}$ [-]
iCO_2	CO_2	0.08	1.01	188.92	0.97	1.26
niCO_2	CO_2	1.29	1.05	188.92	0.59	2.63
iMD_2M	MD_2M	0.32	1.02	26.76	0.94	0.96
niMD_2M	MD_2M	1.23	1.02	26.76	0.50	0.56

of the gas dynamic of NICFD flows and in particular of dense vapor flows. The other two examples show how the user can get practical insights on the design implications of fluid machinery components when they operate with dense vapors.

4.1. Conceptual understanding of non-ideal flows

The working fluids and the reduced inlet conditions selected for this study are summarized in Table 2. The prefix "i" identifies thermodynamic processes occurring in the ideal or dilute gas region, whereas the prefix "ni" is associated to thermodynamic transformations occurring in the non-ideal or dense vapor region. The following considerations can be stated by inspecting Figs. 2 and 3. For both fluid molecules, the dilute vapor region is characterized by moderate values of reduced temperature and low values of reduced pressure. As theoretically predicted, in dilute gas state the value of the compressibility factor is approximately unitary and the value of the isentropic pressure–volume exponent approaches the one of the specific heat capacity ratio computed under ideal gas assumption. On the other hand, the dense gas region, characterized by low values of Z and large gradients of γ_{Pv}, is associated to higher reduced pressure and is located in the proximity of the fluid critical point. In general terms, the more complex is the fluid molecule, the lower is the minimum value assumed by both Z and γ_{Pv} in the dense vapor region, and consequently the higher is the departure with respect to ideal gas behavior. The user can quantify such departure by plugging the averaged value of γ_{Pv} into the generalized isentropic relations provided in [19]. Working fluids made by heavy and complex molecules exhibit a positive slope of the dew line, enabling isentropic transformations spanning from the supercritical



(a) Non-dimensional nozzle shape

(b) Mach number vs. non-dimensional nozzle length

Fig. 4. Converging–diverging nozzles designed for isentropic expansions labeled as iMD_2M and $niMD_2M$, featuring a pressure ratio $P_t/P = 4$.

to the vapor region in the proximity of the saturation curve, characterized by strong non-ideal and possibly non-classical gas dynamic effects, see process $niMD_2M$ in Fig. 3. On the contrary, isentropic expansions of simple fluid molecules in the neighborhood of the critical point entail crossing of the saturation curve, and thus are characterized by the occurrence of two-phase flows. The study of such physical processes is out of the scope of the present work, but the capabilities to perform two-phase flow calculations will be part of a future release of NiceProp.

4.2. Design of converging–diverging nozzles

The second example deals with the preliminary design of converging–diverging nozzles for the two expansion processes labeled as iMD_2M and $niMD_2M$, both at a pressure ratio $P_t/P = 4$. The two nozzles feature a rectangular section with unitary depth, they are designed for a mass flow rate of 1 kg/s and for an inlet flow velocity of 25 m/s and 10 m/s, respectively, to obtain approximately the same inlet Mach number given the two different thermodynamic states. Furthermore, the two nozzle sections share the same inlet and outlet non-dimensional length, i.e.

$$\begin{aligned} 2(x_{\mathrm{throat}} - x_{\mathrm{in}})/y_{\mathrm{throat}} &= 2.3 \\ 2(x_{\mathrm{out}} - x_{\mathrm{throat}})/y_{\mathrm{throat}} &= 1.7 \end{aligned} \tag{10}$$

In other words, the two nozzles feature the same throat location in the non-dimensional space. The resulting non-dimensional nozzle sections designed by NiceProp are shown in Fig. 4(a). The corresponding trend of Mach number computed over the non-dimensional length of the flow devices is displayed in Fig. 4(b).

One can deduce the following considerations from the analysis of the two charts. First, the nozzle designed for the non-ideal flow expansion features a much wider diverging section, as compared to the one expanding MD_2M in dilute gas state. This is a direct consequence of the larger density gradient experienced by the fluid when expanding in the dense vapor region. Such effect must be accounted for when designing turbomachinery components, e.g. supersonic turbine stators. If, for example, a supersonic stator designed to expand an ideal siloxane flow is used to perform a thermodynamic transformation similar to $niMD_2M$, the resulting flow field will be characterized by a strong post-expansion and associated flow deviation, to compensate for the insufficient area variation provided in the blade channel.

Moreover, the two nozzles feature both quantitative and qualitative deviations in the Mach number trend computed along the diverging section. The expansion in dilute gas state shows a monotonically increasing trend of Mach number, whereas process $niMD_2M$ features a local inversion of Mach number during flow acceleration. Such unconventional gas dynamic phenomenon can, for example, reduce the entropy generation due to the shock system formed at the trailing edge of a supersonic stator and can be predicted early in the design process by looking at the local inversion of γ_{Pv} along the prescribed expansion process, see Fig. 5.

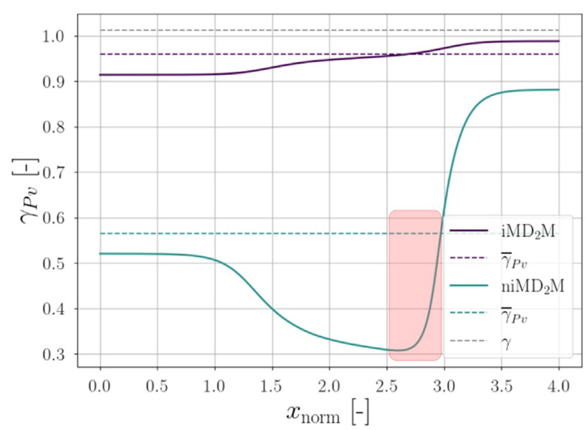
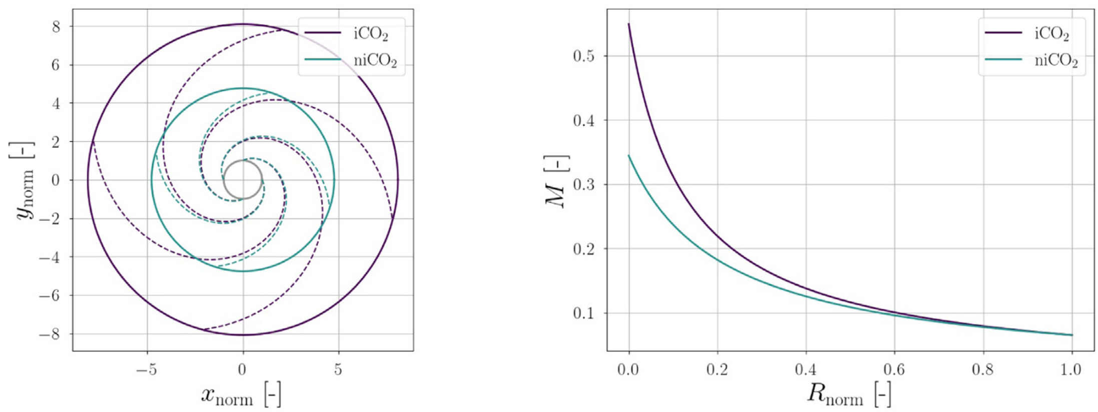


Fig. 5. Isentropic pressure–volume exponent vs. non-dimensional nozzle length. The region of local trend inversion is highlighted in red. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4.3. Design of radial diffusers

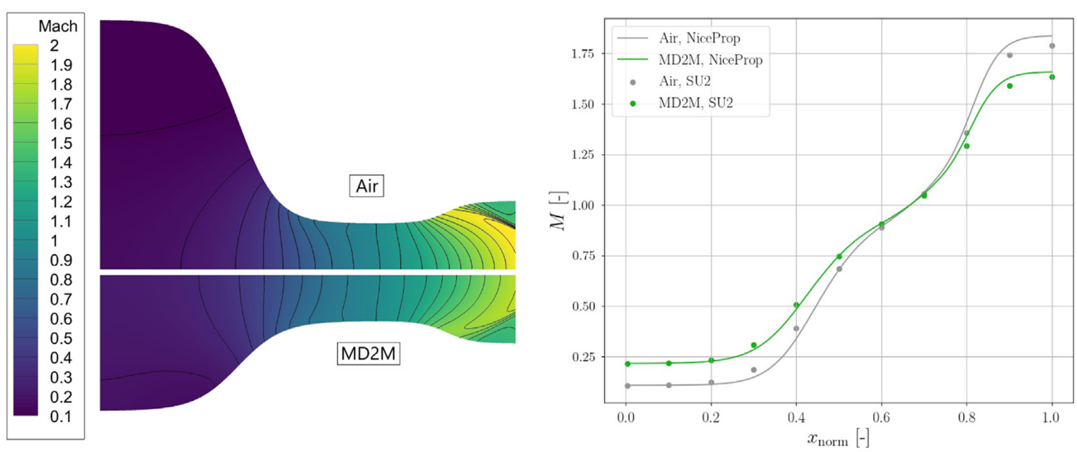
The last example used to demonstrate the capabilities of NiceProp consists in the preliminary design of radial diffusers for the two compression processes labeled as iCO_2 and $niCO_2$, featuring a pressure ratio $P_t/P = 4$. The two diffusers are designed for a unitary mass flow rate and for an outlet flow velocity of 20 m/s and 30 m/s, respectively, to get roughly the same outlet Mach number. The resulting shape of the flow devices and the trend of Mach number computed over the normalized radius are displayed in Fig. 6. It can be noted that the compression of CO_2 in dilute gas state requires a much larger diffuser. The reason thereof is that supercritical CO_2 exhibits a liquid-like flow behavior, characterized by a small density variation over the compression process which ultimately leads to a more compact diffuser design. From a conceptual point of view, as observed for the non-ideal expansion of siloxane MD_2M, the lower the averaged value of γ_{Pv} over the thermodynamic transformation, the higher is the required area variation of the component. Moreover, the limited density



(a) Non-dimensional diffuser shape

(b) Mach number vs. non-dimensional diffuser radius

Fig. 6. Radial diffusers designed for isentropic compressions labeled as iCO_2 and $niCO_2$, featuring a pressure ratio $P_t/P = 4$.



(a) Mach contours computed with SU2

(b) Mach trends along the mean streamline computed with SU2 and NiceProp

Fig. 7. CFD validation of the Mach trends computed by NiceProp for two reference nozzles operating with air and siloxane MD2M.

variation observed for case $niCO_2$ leads to a lower flow deceleration in meridional direction, thus to a lower flow deflection in azimuthal direction, as shown by the dashed lines in Fig. 6(a). A smaller flow angle leads to a shorter flow path throughout the vaneless diffuser and thus to lower losses associated to viscous friction. The diffuser stability characteristics also benefit from the reduction of flow deflection.

4.4. CFD validation

The purpose of the present section is to assess the accuracy of the methods implemented in NiceProp against a more accurate numerical method. The open-source NICFD solver SU2 [28] has been chosen as benchmark for this analysis. The selected test cases consist of two converging–diverging nozzles designed by means of NiceProp for air and siloxane MD_2M in dilute gas state. The flow is simulated by solving the Euler equations using a mesh of approximately 50 k grid points. The thermodynamic properties of the fluid are calculated using the polytropic Peng–Robinson gas model. The boundary conditions used for the CFD simulations are summarized in Table 3. A similar CFD model has been successfully adopted in previous works [29,30].

The Mach number contour obtained with SU2 for the two test cases is shown in Fig. 7(a). As can be observed, the nozzle designed by NiceProp can effectively expand the flow up to supersonic conditions with the prescribed boundary conditions. However, it should be noted that the resulting flow field is not uniform at the outlet section. In order to achieve uniform flow at nozzle outlet, one must design the nozzle with more advanced methods like the method of characteristics [31]. This is however beyond the scope of the software.

Table 3
Boundary conditions used for the CFD simulations.

Fluid	$P_{t,in}$ [bar]	$T_{t,in}$ [K]	P_{out} [bar]	γ [-]
Air	18.925	530.53	3.108	1.4
MD_2M	3.661	611.4	0.915	1.019

The values of Mach number corresponding to the mean streamline are extracted from the CFD results and plotted against the values given by NiceProp. The comparison is displayed in Fig. 7(b). The trends are in very good agreement, demonstrating that NiceProp can be effectively used as a tool to interactively learn and evaluate the impact of NICFD on the design of internal flow devices.

5. Impact

NicePropis targeted to graduate students, researchers and industry professionals dealing with NICFD science and technology. Engineering applications whereby NICFD effects are relevant are numerous and continuously growing, thus the community that can potentially benefit from the use of NiceProp is vast. Since NICFD is a relatively new branch of fluid-mechanics, NiceProp can serve to educate practitioners to the use of a proper terminology, to improve the understanding of non-ideal flows, and to learn about the impact of non-ideal flow effects on the design of fluid machinery components. The use of the software is highly supported by the Knowledge Center on Organic Rankine Cycle technology (KCORC), the community hub of the members from academia and industry dedicated to the promotion of the organic Rankine cycle technology. Moreover, NiceProp can be easily extended and exploited to investigate new research ideas. For example, researchers can utilize the tool to theoretically predict gas dynamic phenomena associated to expansion or compression processes of non-ideal fluid mixtures [32] and two-phase equilibrium flows, that can be eventually studied with more advanced numerical methods and experimental techniques. The study of non-ideal mixtures of fluids and two-phase flows has many practical implications for the development of novel energy conversion systems.

6. Conclusions

The paper describes the object-oriented Python program NiceProp, which is meant for interactively learning non-ideal compressible fluid dynamics. The software can be used to perform thermodynamic studies and analysis of expansion and compression processes of ideal and non-ideal flows. Furthermore, converging–diverging nozzles, conical and radial diffusers operating in the dilute gas and dense vapor regimes can be easily designed and flow features analyzed. By using the tool in a systematic way, the user can quickly develop conceptual understanding of non-ideal flows, as well as gain practical insights on the design of internal flow devices operating with such kind of flows. The current version of the tool implements models for dense vapors, however models for two-phase equilibrium flows and non-ideal fluid mixtures can be easily added in future releases thanks to the modular structure of the software.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. Input file structure

************************** BASIC SETTINGS **************************
Working fluid
CO2
Equation of state: 'PR', 'SRK', 'HEOS' or 'REFPROP'
REFPROP
Thermodynamic plane: 'Ts' or 'PT'
PT
***************** ISENTROPIC TRANSFORMATION ******************
Process(es): 'compression' or 'expansion' or 'None'
compression
Do you want to design nozzle/diffuser? Y/N
Y
Total-to-static volumetric flow ratio
0.0
Total-to-static pressure ratio
4.0
Inlet state definition: 'Ts' or 'PT'
Ts Ts
Inlet state definition: first input
1.01 1.05
Inlet state definition: second input
1.70 1.10
Label(s) associated to the thermodynamic process(es)
iCO_2 $niCO_2$
Nozzle geometry is provided as input? Y/N
N
*********************** COMPONENT DESIGN ***********************
Mass flow rate [kg/s]
1.0 1.0
Flow velocity [m/s] at inlet for nozzle, at outlet for diffuser
20.0 30.0
Nozzle/diffuser geometry
radial
********************* CONTOUR PLOT SETTINGS *********************
Number of grid points on x and y axes for Ts/PT contour plots
1000
Boundaries of contour plots along reduced T axis
0.60 2.00
Boundaries of contour plots along reduced s axis
0.75 2.00
Boundaries of contour plots along reduced P axis
0.50 5.50

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