NON-IDEAL COMPRESSIBLE-FLUID DYNAMICS SIMULATION WITH SU2: NUMERICAL ASSESSMENT OF NOZZLE AND BLADE FLOWS FOR ORGANIC RANKINE CYCLE APPLICATIONS

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ABSTRACT

The growing interests towards Organic Rankine Cycle (ORC) turbo-machinery calls for reliable and well-established simulation and design tools, including Computational Fluid Dynamics (CFD) software, accounting for non-ideal thermodynamic behaviour in close proximity to the liquid-vapour saturation curve and critical point, as well as two-phase properties. SU2, an open-source CFD solver originally developed at Stanford University, Palacios et al. (2013, 2014), was recently extended to deal with non-ideal thermodynamics, including state-of-the-art multi-parameter equations of state implemented in the FluidProp library, Colonna and van der Stelt (2004), and it is now in the process of becoming a reliable simulation tool for academic and industrial research on ORC machinery. The investigation of SU2 performances in connection with the numerical simulation of steady nozzle and turbine flows of interest for ORC applications are provided. Numerical simulations refer to both inviscid and viscous flow, with diverse thermodynamic (ideal gas, Van der Waal gas, Peng- obinson Stryjek-Vera, Span-Wagner multi-parameter equation of state) and turbulence (Spalart-Allmaras, SST-k) models. Considered geometries include straight axis planar nozzle, and a typical ORC turbine blade passage.

1. INTRODUCTION

Nowadays applications involving non-ideal compressible flows can be found in numerous industrial problems and are spread over heterogeneous fields. During the last decade Organic Rankine Cycle turbo-machinery became of utmost importance for the future design of highly efficient energy production systems. In practical applications the ORC machinery make use of particular fluids that, under certain conditions of pressure and density, may show non-ideal thermodynamic behaviour. For these fluids the ideal gas law is proved to fail in describing accurately the thermodynamic behaviour when pressure and temperatures are close to the liquid-vapour saturation curve, in the region near the critical point. The rising of non-ideal compressible fluid phenomena thus calls for more complex equations of state, like for instance the Van der Waals or the Peng-Robinson Stryjek-Vera equation of state or the multi-parameter equation of state. These complex gas models are of utmost importance and can possibly provide a more accurate description of the thermodynamic behaviour that characterizes these fluids. Nowadays the community can only rely on a few computational tools capable of dealing with real fluid flows. One of these tools is *zFlow*, developed by S. Rebay and P. Colonna, a solver suitable for compressible inviscid dense gas flows where an hybrid Finite-volume/Finite-element discretization scheme is adopted, Colonna et al. (2002). Such code has been already proved to provide accurate predictions of the flow field inside ORC three-dimensional radial turbine. Today the academic community and the industry desire for a more reliable and well-maintained investigation tool, to prove the accuracy of the state-of-the-art equation of state and to foster the design of new, more efficient, power production systems. This tool should serve as a framework from which users can start developing their own real-gas models, including new numerical algorithms and customized features, without worrying about the maintenance of the overall structure. The Stanford University Unstructured (SU2) software suite recently became a promising candidate for this role. SU2 is a popular open-source platform for solving multi-physics PDE problems and PDE-constrained optimization problems on general, unstructured meshes. The core of SU2 is a Reynolds-averaged Navier-Stokes (RANS) solver dedicated to the simulation of compressible, turbulent flows. The capabilities of this solver are various and their number is growing quickly as developers from the international team contribute to improve the code, providing new features and extending its capabilities. A joint research team composed by researchers from Delft University of Technology, from the Politecnico di Milano, and from the Stanford University recently undertook a collaborative effort to bring the SU2 at the cutting-edge for non-ideal compressible fluid-dynamics (NICFD) simulation, Vitale et al. (2015),, extending SU2 capabilities to a wider range of pertinence with the inclusion of the Van der Waals and the Peng-Robinson Stryjek-Vera equation of state. The early work has been lately extended with the inclusion of the FluidProp, Colonna and van der Stelt (2004), thermodynamic library which opens the path to the exploitation of the state-of-the-art multi-parameter equation of state. The SU2 suite already included a library for thermo-physical properties of reacting non-equilibrium flows, such as those involving combustion, though a computational framework for NICFD simulation was completely missing. In compliance with the open-source philosophy of the project all the modifications are made available to the community, thus contributing to promote a worldwide access to state-of-the-art analysis tool for NICFD. The actual characteristics of dense vapours, supercritical flows and compressible two-phase flows, in close proximity to the saturation curve near the critical point, entail that the thermodynamic behaviour of the fluid differs considerably from that described by the perfect gas law and, under particular conditions, they may even exhibit non-classical gas-dynamic phenomena. The nature of this particular phenomena is related to the value of the fundamental derivative of gas-dynamics Γ. A non-monotonic Mach number trend along expansion is typical for values of Γ enclosed between 0 and 1, while negative values may bring to the occurrence of inverse gas-dynamics phenomena such as rarefaction shock waves, splitting waves or even composite waves. Heavy complex molecule in the vapour region are expected to show inverse gas-dynamics behaviour, Colonna et al. (2007), and recently two-phase rarefaction shock waves have been recognized as physically realizable close to the critical point of simple compounds, Nannan et al. (2014).

The paper is organized as follows: the first part recalls a brief description of the governing equations for an arbitrarily complex fluid at equilibrium condition and a short review of the numerical method implemented in the SU2 suite. In the second part we present some exemplary results involving simple geometries such as straight axis planar nozzles and a typical ORC turbine blade passage.

2. NUMERICAL MODEL

This section outlines the most distinguishing features of the SU2 solver for non-ideal compressible fluid flows. We first remember that, differently from past attempts and commercial alternatives, the modular and open-source infrastructure of the SU2 suite is largely suitable to build upon the existing flow model new knowledge and methods for fundamental and applied studies for non-ideal fluid flows. Currently, SU2 solves the equilibrium compressible RANS equations, Landau and Lifshitz (1993), by levering on a general formulation enabling the use of arbitrary thermo-physical models. The system of PDE equations including the inviscid and viscous terms is written as

$$\partial_t U + \nabla \cdot \vec{F}^c - \nabla \cdot \vec{F}^v = Q \quad \text{in } \Omega,\, t > 0 \tag{1}$$

Equation (1) describes how mass, momentum and energy evolve in a control domain. $\vec{U}$ symbolizes the vector of conservative variables, i.e. $\vec{U} = (\rho, \rho v_1, \rho v_2, \rho v_3, \rho E)^T$, where ρ is the fluid density, E is the total energy per unit mass, and $\vec{v} = (v_1, v_2, v_3) \in \mathbb{R}^3$ is the flow velocity in a Cartesian coordinate system. The imposition of the boundary conditions follows the approach proposed in Guardone et al. (2011) to automatically detect inflow/outflow boundaries for hyperbolic systems. Notably the convective and viscous fluxes are given by

$$\vec{F}_i^c = \begin{pmatrix} \rho v_i \\ \rho v_i v_1 + P\delta_{i1} \\ \rho v_i v_2 + P\delta_{i2} \\ \rho v_i v_3 + P\delta_{i3} \\ \rho v_i H \end{pmatrix}, \quad \vec{F}_i^v = \begin{pmatrix} \cdot \\ \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ v_j \tau_{ij} + k_{\text{tot}} \partial_i T \end{pmatrix}, \quad i = 1, \ldots, 3 \tag{2}$$

P is the static pressure, T is the temperature, H is the total enthalpy, δ_{ij} is the Kronecker delta function, and the viscous stresses can be compactly written as $\tau_{ij} = \mu_{tot}\left(\partial_j v_i + \partial_i v_j - \frac{2}{3}\delta_{ij}\nabla \cdot \vec{v}\right)$. The total viscosity and the total thermal conductivity result from a molecular, μ_{mol},k_{mol} and a turbulent, μ_{tur}, k_{tur} contribution. Convective fluxes are properly reconstructed by means of the generalized Roe's approximate Riemann solver (ARS) proposed in Montagne and Vinokur (1990). Second-order accuracy is resolved using a Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) approach, van Leer (1979), with gradient limitation. On the other hand, viscous fluxes are evaluated by averaging the flow variables, flow derivatives, and transport properties at two neighbouring cells whereas the *Thin Shear-Layer* approximation, Blazek (2005), is employed for gradient calculation.

For pure fluids and mixture of given composition in a stable equilibrium state the thermodynamic state can be retrieved by using ρ and internal energy e as follows

$$\rho = U_1, \quad e = \frac{U_5}{U_1} - \frac{(U_2 + U_3 + U_4)^2}{2U_1^2} = E - \frac{\|v\|^2}{2}. \tag{3}$$

The required thermo-physical quantities are conveniently expressed as a function of the ρ, e, i.e. $P = P(\rho, e) = P(U), T = T(\rho, e) = T(U), \mu_{\text{mol}} = \mu_{\text{mol}}(\rho, T(\rho, e)) = \mu_{\text{mol}}(U), k_{\text{mol}} = k_{\text{mol}}(\rho, T(\rho, e)) = k_{\text{mol}}(U)$. The SU2 embeds polytropic models (Van der Waals and Peng-Robinson) for rough and quick estimate of non-ideal flows properties. The other properties characterizing the fluid such as the specific heat capacity C_p and all the transport quantities can be conveniently expressed as

$$\begin{aligned} \mu_{\text{mol}} &= \mu_{\text{mol}}(\rho, T) = \mu_{\text{mol}}(\rho, T(\rho, e)) = \mu_{\text{mol}}(U), \\ k_{\text{mol}} &= k_{\text{mol}}(\rho, T) = k_{\text{mol}}(\rho, T(\rho, e)) = k_{\text{mol}}(U), \\ C_p &= C_p(P, T) = C_p(P(\rho, e), T(\rho, e)) = C_p(U). \end{aligned} \tag{4}$$

For more accurate predictions the SU2 embedded thermo-physical library was recently extended with the inclusion of the FluidProp software, Colonna and van der Stelt (2004), a general purpose thermo-physical database originally accomplished at Delft University of Technology. FluidProp contains several thermo-physical models and provides easy access to the quantities necessary for SU2 simulation, with possibility of handling look-up table interpolations Pini et al. (2014) to fasten the calculation. This opens the path to a wide variety of new capabilities: the properties of fluids –such as viscosity and thermal conductivity– whose thermodynamic state is characterized by a value of pressure and temperature close to the liquid-vapour saturation curve in the region near the critical point, can now be computed with a higher level of accuracy.

The aforementioned non-ideal fluid models now available for SU2 make it possible to represents non-ideal and non-classical phenomena such as rarefaction shock waves or compression fans. Beyond the embedded thermodynamic models, the high flexibility of SU2 and the re-usable thermodynamic infrastructure allows for the future implementation of novel fluid model.

This more general approach calls then for a reformulation of the equations involved by the numerical method. Indeed the ideal gas assumption does apply no more and a general formulation can be obtained from the spectral decomposition of the Roe's averaged state Jacobian. By means of the Roe averaging procedure (5), it follows that a supplemental condition arises (6), namely:

$$\left(\vec{F}_{\mathrm{i}}^{c} - \vec{F}_{j}^{c}\right) = \bar{A}\left(U_{\mathrm{i}} - U\mathrm{j}\right), \quad \bar{A} = A(\bar{U}) \tag{5}$$

$$\bar{\chi}(\rho_{\mathrm{i}} - \rho_{\mathrm{j}}) + \bar{\kappa}(\rho_{\mathrm{i}}e_{\mathrm{i}} - \rho_{\mathrm{i}}e_{\mathrm{j}}) = (P_{\mathrm{i}} - P_{\mathrm{j}}), \tag{6}$$

where $\bar{\chi}$ and $\bar{\kappa}$ are the average of these two thermodynamics quantities defined in eq. (7) and (8).

$$\chi = \left(\frac{\partial P}{\partial \rho}\right)_{\rho e} = \left(\frac{\partial P}{\partial \rho}\right)_{e} - \frac{e}{\rho}\left(\frac{\partial P}{\partial e}\right)_{\rho} \tag{7}$$

$$\kappa = \left(\frac{\partial P}{\partial \rho e}\right)_{\rho} = \frac{1}{\rho}\left(\frac{\partial P}{\partial e}\right)_{\rho} \tag{8}$$

For a PIG fluid this last condition is automatically satisfied as χ equals to zero and κ is constantly equal to $\gamma - 1$. On the other hand, using a NICF model only one relation (6) is provided for the two unknowns $\bar{\chi}$ and $\bar{\kappa}$. Therefore, the Roe-average state remains uniquely defined if and only if a proper closure condition is given.

3. RESULTS

In this section we present some exemplary test case in order to show the reliability of the SU2 suite and to highlight some typical application which may take advantages from the SU2 extended thermo-dynamic library. The considered test cases include simple geometries such as straight axis two-dimensional planar nozzles and a typical ORC turbine blade passage.

3.1 2-D TROVA nozzle

The TROVA (Test Rig for Organic Vapors) experimental facility was built at Laboratorio di Fluidodinamica delle Macchine (LFM) of Politecnico di Milano, Spinelli et al. (2012), and Guardone and Dossena (2012), in collaboration with Turboden s.r.l. and within the frame of the project Solar. In this section we show the flow field predicted by SU2 for a MDM fluid at operating condition listed in table 1: MDM properties, such as thermal conductivity or viscosity, are assumed to be constant through the nozzle. Values are given for the fluid at the inlet conditions and were computed using FluidProp. Results for three different fluid model, namely the polytropic ideal gas law, the polytropic Van der Waals and the polytropic Peng-Robinson Stryjek-Vera from the embedded SU2 thermo-dynamic library, are compared to show how a different level of accuracy in the description of the fluid behaviour may bring to different results. The domain represents a planar two-dimensional straight axis nozzle discharging into a reservoir: the computational grid is an hybrid mesh, hexahedrons were used to describe the boundary-layer region while tetrahedrons to discretize the core region and the reservoir. With reference to Fig 1: a no-slip condition is applied along nozzle wall and on the vertical wall in $x \approx 0.18$, symmetry condition is imposed at the centreline and at the upper boundary of the reservoir. Inlet and outlet conditions are resumed in table 1. The grid in the boundary layer region is extremely refined: this is due to the fact that properties needed for the computation of the first cell height–such as kinematic viscosity–are difficult to determine accurately for the

Fluid	MDM
Gas Constant	35.152 $(J/K/kg)$
Specific heat ratio	1.0125
Critical temperature	564.1 $^\circ K$
Critical pressure	1415000 Pa
Acentric factor	0.529
Total inlet temperature	526.35 $^\circ K$
Total inlet pressure	400000 Pa
Static outlet pressure	1000 Pa
Molecular viscosity	1.376E-5 $Pa \times s$
Thermal conductivity	0.04728 $W/m/K$
Turbulence model	SST-kω and SA
Spatial scheme	Upwind generalized Roe 1$^{\text{nd}}$ order

Table 1: Test conditions for the 2D TROVA nozzle simulation.

involved fluid. Indeed the first cell height for this test case is $\approx 1e^{-7}[m]$–flow involving air in standard condition requires $\approx 1e^{-5}[m]$–. The nozzle is studied when the discharge occurs in off-design conditions, namely when the coefficient of expansion is 5.58 (design conditions correspond indeed to 10), in this test case the nozzle is then operating in an under-expanded regime. The predicted flow-field is shown in figure 1: the upper half of the picture refers to a grid composed by $\approx 75k$ elements while Mach contours in the lower half is related to a $\approx 180k$ cells mesh. This result was obtained using the ideal gas law to describe the fluid thermodynamic behaviour and the SST-$k\omega$ for modelling turbulence. At the discharge section a Prandtl-meyer expansion occurs: the flow is turned outwards and redirected towards the reservoir wall, where a symmetry boundary condition holds. The supersonic flow hence hits the boundary fostering the rise of a compression shock-wave: a system of reflected shock-wave then propagates through the reservoir. Figure 1 shows how a more refined discretization of the reservoir is needed in order to represent the wave reflecting system with a higher level of resolution. This was expected since a numerical scheme of the first order is highly dissipative and hence strongly dependent on the grid spacing: shock-wave in the coarser mesh is indeed smeared out moving along the nozzle axis. Mach and pressure trends along the centreline for the three different equation of state, computed using the SST-$k\omega$ turbulence model, are reported in figure 2 and 3.

3.2 2-D ORCHID nozzle

The ORCHID (Organic Rankine Cycle Hybrid Integrated Device) is an experimental facility being constructed at the Aerospace Propulsion and Power (APP) Lab. of the Delft University of Technology. It will be used to perform gas dynamic studies of non-ideal expansions and performance comparisons of high-speed ORC turbomachinery. The facility has been set up in collaboration with Robert Bosch GmbH (Solar ORC turbogenerator for zero-energy buildings) and by Dana-Spicer Corp (Mini-ORC turbogenerator for combined cycle powertrains). In this section we show a flow field simulated by SU2 for the linear siloxane hexamethyldisiloxane (MM); namely one of the working fluids considered in the design of the ORCHID with simulation parameters and set values specified in Table 2. RANS equations are solved with the slip condition at the walls and symmetry along the mid-plane. The FEQ Helmholtz equation of state implemented in the FluidProp thermo-dynamic library is used to model the fluid behaviour, the result is compared to the output from the integral balance equations for an adiabatic flow and a steady oblique shock wave. The test case is presented in Figure 4; a two-dimensional converging-diverging nozzle generated with a MoC code, Guardone and Dossena (2012), with a model placed 18 mm from the throat with a flow turning angle $\theta = 20^\circ$ along the centreline. Figure 5 depicts the terminology used, with β corresponding to the oblique shock wave angle and V to the velocity before and after the shock. The shock wave resulting from the CFD computation is 45.0 $^\circ$ and is reflected off the nozzle profile wall, subsequently

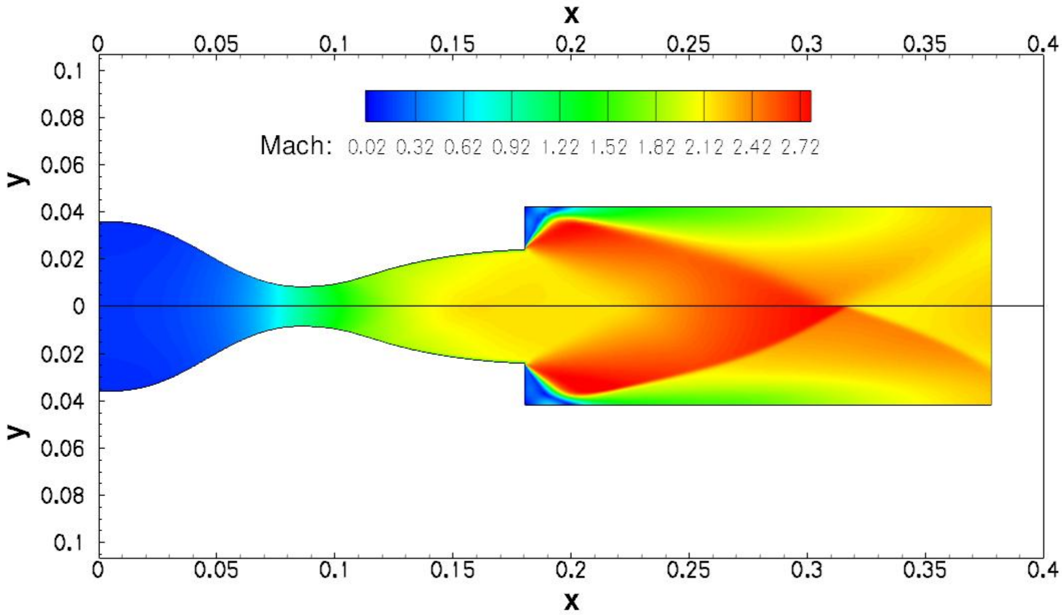

Figure 1: Mach contour in TROVA nozzle using polytropic ideal gas equation of state and SST-$k\omega$ turbulence model for two different level of mesh refinement: respectively $\approx 74k$ elements (upper side) and $\approx 180k$ elements (lower side). Axis refers to dimensional length [m].

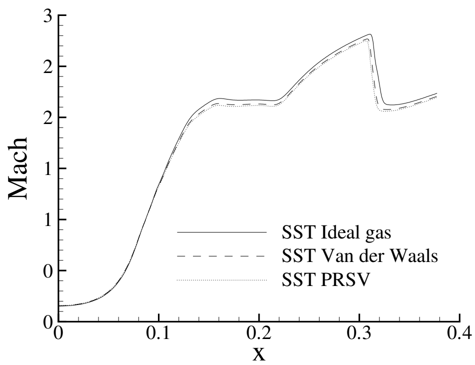

Figure 2: Comparison of Mach number trends along the centreline.

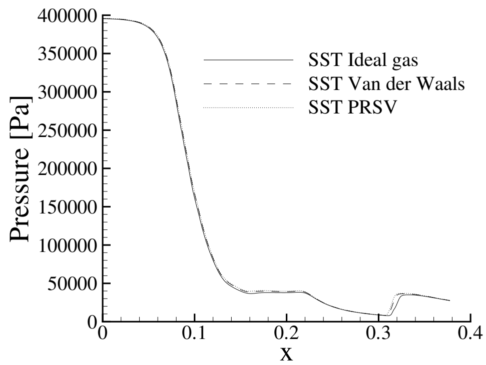

Figure 3: Comparison of pressure trends along the centreline.

Fluid	MM
Thermodynamic model	FEQ Helmholtz
Critical temperature	518.75 K
Critical pressure	19.39 bar
Total inlet temperature	525.15 K
Total inlet pressure	18.4 bar
Spatial scheme	Upwind generalized Roe 2nd order
Turbulence model	SST-kω
Inlet turbulence intensity	0.001
Reynolds Number Throat	1.642E6
Spatial scheme	Upwind generalized Roe 2nd order

Table 2: Main parameters of the 2D ORCHID supersonic nozzle simulation.

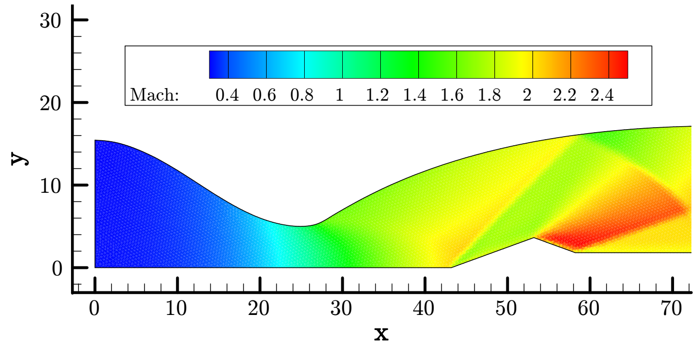

Figure 4: Mach contours of the 2D nozzle.

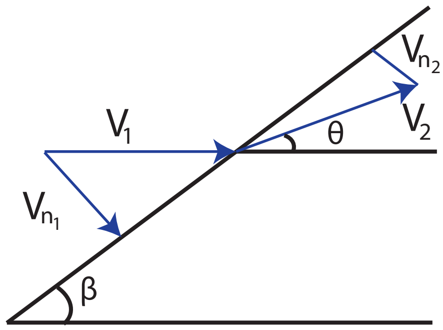

Figure 5: Oblique Shock Wave Angles and Vectors.

cutting the expansion fan that is generated from the back of the model. It is well known that the conditions across the surfaces of discontinuities are governed by the integral conservation equations. The jump conditions across a steady shock-wave for the continuity, momentum and energy equations cannot be solved with a simple closed-form expression as is the case for an ideal gas. The Rankine-Hugoniot relations are rendered obsolete and thus, for a non-ideal gas which uses more complicated equations of state, an iterative calculation procedure is employed to obtain the thermodynamic change across a shock wave and is given by Grossman (2000). It is now possible to determine the relationship between the M_1-β-θ variables and when providing inputs such as θ, V_1, P_1 and ρ_1, properties after the shock may be calculated. This allows calculation of relevant data such as shock strength, angle and the location along the mid-plane where detachment occurs, while maintaining relatively fast computational times. The resulting β is 44.3° and represents a 1.5 % deviation in the solution compared to the results in Figure 4 above.

3.3 Supersonic ORC turbine stator

In this test-case the capabilities of the new NICFD solver are tested in predicting the flow feature of a supersonic ORC turbine cascade. The calculations are performed using the inviscid solver, the SA and the SST-$k\omega$ turbulence models. Table 3 summarizes the main inputs for the solver.

Figure 6 plots the Mach contour of the simulation using the SST-$k\omega$, and, as can be noticed, the flow field is characterized by intense shocks and expansion fan interactions at the outlet. It is important to predict these phenomena with high accuracy because they generally represent the main source of fluid-dynamic losses for these particular applications. As can be seen indeed from Fig. 7 no distinctions can be appreciated in the pressure distribution trends plotted for the three different simulations. Figure 8 confirms the predominance of supersonic effect on the flow solutions, and a very low discrepancy can be appreciated on the flow Mach number trend at the outlet section.

4. CONCLUSIONS

In this paper SU2 CFD suite was considered as a possible candidate for representing a reliable investigation tool for the study and for the design of Organic-Rankine Cycle turbo-machinery. SU2 simulating capabilities were recently extended to real gas flows by the inclusion of an embedded collection of fluid models, which comprehend three different equation of state–polytropic ideal gas, polytropic Van der Waals and polytropic Peng-Robinson Stryjek-Vera–for the description of fluid behaviour and also by the inclusion of the FluidProp thermo-physical library.

Fluid	MDM
Specific heat ratio	1.0214
Total inlet temperature	545.17 $^\circ K$
Total inlet pressure	800000 Pa
Static outlet pressure	10000 Pa
Molecular viscosity	1.0461E-5 $Pa \times s$
Thermal conductivity	0.028085 $W/m/K$
Turbulence model	SST-kω and SA
Inlet turbulence intensity	0.05
Spatial scheme	Upwind generalized Roe 2nd order

Table 3: Test conditions for the 2D supersonic stator.

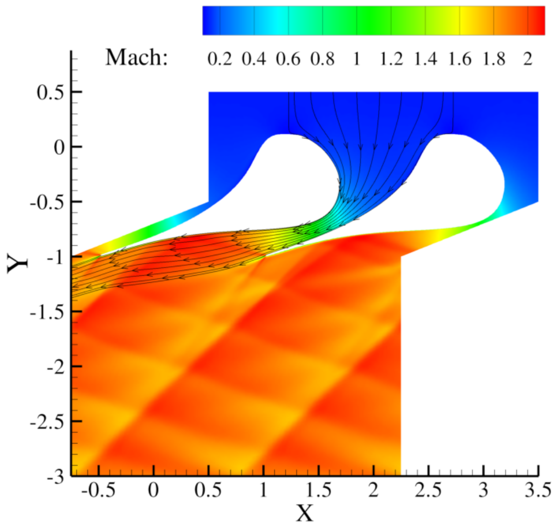

Figure 6: Mach flow field of the 2D supersonic stator fusing the SST-$k\omega$ turbulence model. Units on the axis are scaled due to industrial secrecy.

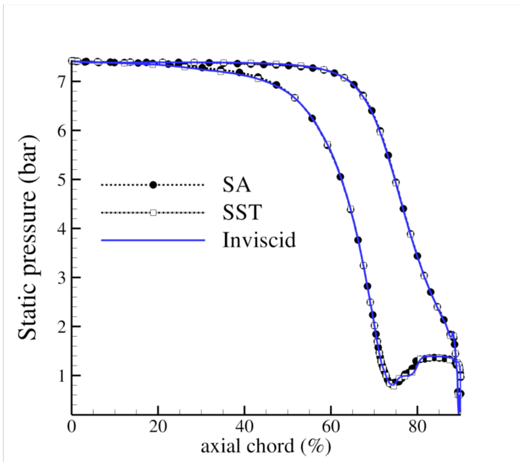

Figure 7: Pressure distribution around the blade profile for the inviscid case and with SA and SST turbulence models.

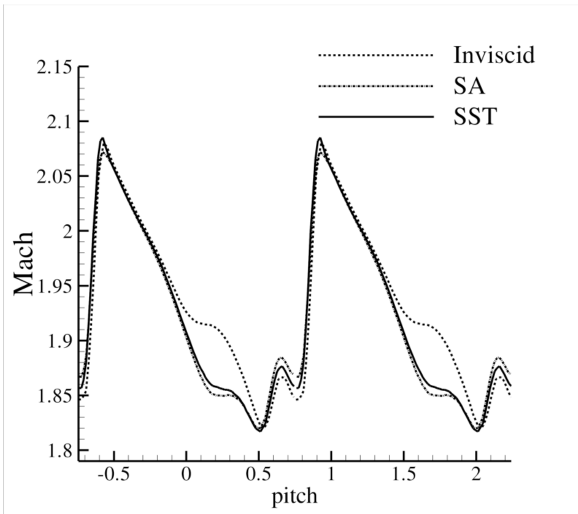

Figure 8: Mach trend at the outlet for the inviscid case and with SA and SST turbulence models.

Within the aim of SU2 it is possible to manage non-ideal compressible flows that may exhibit non-classical gas-dynamic phenomena. This include fluid flows that slightly depart from an ideal behaviour but also fluid flows that give birth to rarefaction shock-waves and compression fans. The open-source trait opens the path to a wide range of possibilities: the integration of new software packages devoted to real gas applications is easily achievable within the SU2 framework. In this paper we showed that SU2 is already capable of tackling problems that engineers or researchers may face in typical ORC applications: simulation involving geometries of utmost importance such as nozzles and a typical ORC turbine blade passage were carried out. Different equation of state were used to describe the thermodynamic behaviour of fluids characterized by a highly complex molecular structure and using both first and second order numerical schemes.

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ACKNOWLEDGEMENT

The research is partially funded by the European Research Council under Grant ERC Consolidator 2013, project NSHOCK 617603.