

Field inversion for data-augmented RANS modelling in turbomachinery flows

Original

Field inversion for data-augmented RANS modelling in turbomachinery flows / Ferrero, A.; Iollo, A.; Larocca, F.. - In: COMPUTERS & FLUIDS. - ISSN 0045-7930. - ELETTRONICO. - 201:(2020), p. 104474.
[10.1016/j.compfluid.2020.104474]

Availability:

This version is available at: 11583/2803272 since: 2020-03-23T11:09:47Z

Publisher:

Elsevier Ltd

Published

DOI:10.1016/j.compfluid.2020.104474

Terms of use:

This article is made available under terms and conditions as specified in the corresponding bibliographic description in the repository

Publisher copyright

Elsevier postprint/Author's Accepted Manuscript

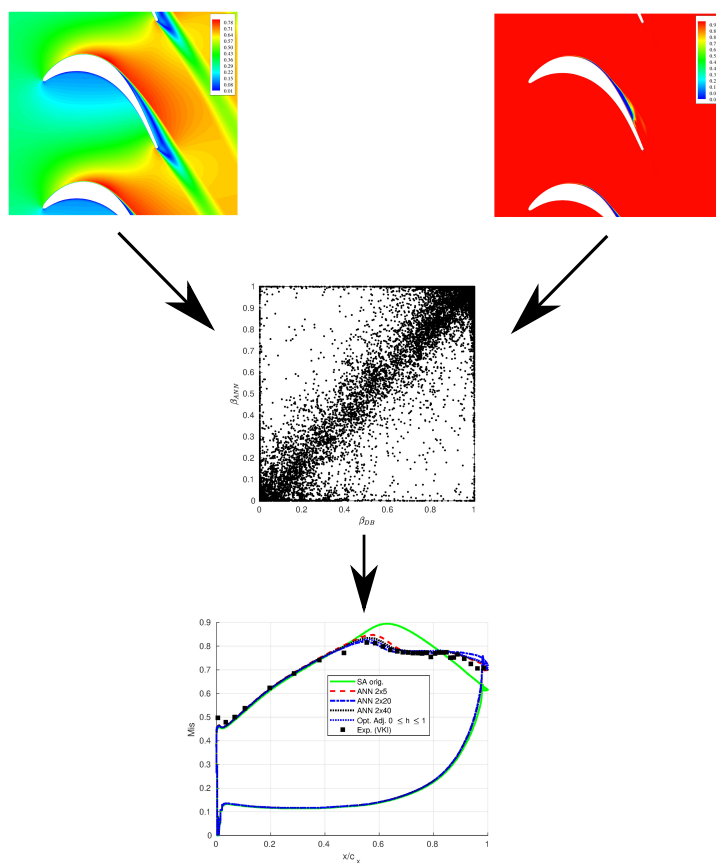
© 2020. This manuscript version is made available under the CC-BY-NC-ND 4.0 license
<http://creativecommons.org/licenses/by-nc-nd/4.0/>. The final authenticated version is available online at:
<http://dx.doi.org/10.1016/j.compfluid.2020.104474>

(Article begins on next page)

Graphical Abstract

Field inversion for data-augmented RANS modelling in turbomachinery flows

Andrea Ferrero, Angelo Iollo, Francesco Larocca



Highlights

- The field inversion approach is investigated for improving RANS models in turbomachinery flows
- Working conditions characterised by transition and separation are considered
- Some approaches to improve the robustness of the method are proposed
- The augmented RANS model includes an Artificial Neural Network which acts as an intermittency term
- The predictive ability of the method is investigated for several working conditions on different geometries

Field inversion for data-augmented RANS modelling in turbomachinery flows

Andrea Ferrero^{a,*}, Angelo Iollo^{b,c,d}, Francesco Larocca^a

^a*Politecnico di Torino, 10129 Torino, Italy*

^b*Memphis Team, INRIA, F-33400 Talence, France*

^c*Univ. Bordeaux, IMB, UMR 5251, F-33400 Talence, France*

^d*CNRS, IMB, UMR 5251, F-33400 Talence, France*

Abstract

Turbulence modelling in turbomachinery flows remains a challenge, especially when transition and separation phenomena occur. Recently, several research efforts have been devoted to the improvement of closure models for Reynolds-averaged Navier-Stokes (RANS) equations by means of machine learning approaches which make it possible to extract the knowledge hidden inside the available high-fidelity data (from experiments or from scale-resolving simulations). In this work the use of the field inversion approach is investigated for the augmentation of the Spalart-Allmaras RANS model applied to the flow in low pressure gas turbine cascades. As a first step, the field inversion method is applied to the T106c cascade at two different values of Reynolds number (80000-250000): an adjoint-based gradient method is employed in order to minimise the prediction error on the wall isentropic Mach number distribution. The data obtained by the correction field are then analysed by means of an Artificial Neural Network (ANN) which makes it possible to generalise the correction by finding correlations which depend on physical variables. A study on the definition of the input variables and on the architecture of the ANN is performed. Different kind of corrections are evaluated and a particularly robust correction factor is obtained by limiting the range of the correction in the spirit of intermittency models. Finally, the ANN is introduced in an augmented version of the Spalart-Allmaras model which is tested on the T106c cascade (for values of the Reynolds number

*Corresponding author

Email address: andrea_ferrero@polito.it (Andrea Ferrero)

not considered during the training) and for the T2 cascade. The prediction ability of the method is investigated by comparing the numerical predictions with the available experimental data not only in terms of wall isentropic Mach number distribution (which was used as goal function during the field inversion) but also in terms of mass averaged exit angle and kinetic losses.

Keywords: Field inversion, Machine learning, Turbulence modelling, Turbomachinery

1. Introduction

The recent trends in the simulation of the flow field inside aerospace propulsion systems are characterised by a growing interest towards high-fidelity simulations which have become feasible thanks to a significant increase in the available computational power. This paves the way to the possibility of understanding complex physical effects which characterise turbulence and combustion phenomena in modern engines. The ability to understand and control these effects can be exploited to increase the performance and reduce the emissions of existing propulsion systems. However, scale-resolving simulations (like for example Direct Numerical Simulations (DNS) or Large Eddy Simulations (LES)) cannot be easily integrated in the design process of industrial components. This is due to two main reasons: computational cost and difficulty to manage the results. It is clear that in the first steps of a design process several configurations must be investigated and the use of high-fidelity simulations in this phase would have a prohibitive cost. For this reason, less expensive approaches like RANS equations will be probably used for several years. As far as the management of the results is concerned, LES and DNS usually generate a huge amount of data for each simulation: in order to extract the useful information required by the design process it would be necessary to perform a complex post-process step. For example, even the computation of the average field from unsteady DNS data is not trivial because it is not known a-priori the extension of the time window required to get statistically converged results: several examples of low frequency phenomena which make difficult to compute the average field can be found in the literature, even looking to simple test cases, and special strategies to estimate the statistical error should be used [1]. A review of the current state of the art for high-fidelity simulations in turbomachinery was proposed by Sandberg and Michelassi [2].

Recently, several research efforts have been devoted to the development of machine learning algorithms for all those applications in which a large amount of data must be processed. In particular, several recent works in the literature have been devoted to the use of machine learning techniques to analyse high-fidelity data from experiments or high-fidelity numerical simulations. The idea behind most of these recent works is to get the physical insight hidden in the data and use it to develop or improve low order data-driven models. An example of this philosophy is represented by the work of Xie et al. [3] who proposed a filtered reduced order model with a data-driven closure. Dupuis et al.[4] proposed an approach in which traditional surrogate models and machine learning are combined to improve the prediction of the flow on airfoils which work in subsonic or transonic conditions. Margheri et al.[5] performed a study on the epistemic uncertainty of some popular RANS models and used a generalised Polynomial Chaos response surface to perform the calibration of the model coefficients in the spirit of data assimilation strategies. In [6] the Proper Orthogonal Decomposition approach is used in a discontinuous Galerkin (DG) finite element framework [7] together with a domain decomposition strategy [8] to learn empirical local bases which are used to reduce the simulation cost of the flow field in gas turbines.

An alternative path was followed by Raissi and Karniadakis [9] who proposed an approach to identify the partial differential equations which govern a set of data: they applied the algorithm to an example in which they recovered the Navier-Stokes equations used to generate the database but the same approach could be used on experimental data to recover turbulence models. While the work of Raissi and Karniadakis [9] aims at discovering the full governing model, several works focus on the improvement of existing models. For example, Wang et al. [10] developed a machine learning strategy to predict the discrepancy in RANS modelled Reynolds stresses starting from DNS data. Weatheritt et al.[11] proposed the use of Gene Expression Programming to identify new expressions for the stress-strain relationship. Promising results were obtained with this technique on high pressure turbines [12]. Duraisamy et al. [13, 14] proposed a strategy based on field inversion and machine learning which allows to improve the prediction ability of RANS models. This approach is exploited in the present work in order to improve RANS modelling for low pressure gas turbine cascades.

Machine learning techniques have been investigated also on multiphase flows [15, 16], combustion [17, 18, 19] and engine modelling [20, 21]. Finally, a comprehensive review of the machine learning techniques proposed for the

improvement of turbulence modelling can be found in [22].

The paper is organised as follows. In Section 2 the original RANS model is presented. In Section 3 the methods used for the discretisation of the equations are described. In Section 4 the field inversion approach is described and it is then applied to the T106c gas turbine cascade in Section 5. The data obtained by the field inversion are analysed by means of machine learning techniques in Section 6 in order to generalise the obtained results. Finally, the improved RANS model is tested on the T106c and on the T2 cascades in Section 7.

2. Physical model

This work is devoted to the prediction of the compressible turbulent flow in 2D turbine cascades. The study starts from the Spalart-Allmaras (SA) model implemented for compressible equations, following the guidelines of [23]. This model is widely used in the literature for fully turbulent flows. However, the model is not suitable for the prediction of transitional flows at low Reynolds numbers. The original model gives the possibility to impose the transition location (by means of the trip term f_{t1} defined in [23]) but this choice is rarely followed in the literature because in general the location of transition is not known a-priori. Furthermore, when the transition trip term f_{t1} is used a second term f_{t2} for delaying natural transition (and making the trip term f_{t1} effective) is also activated. Further details on the effects of the term f_{t2} in the prediction of the flow around the T106c cascade can be found in [24].

In the present work the SA model is used without the trip terms f_{t1} and f_{t2} . With this choice the model is expected to work fine for high Reynolds numbers but to fail in predicting transition and separation at low values of Reynolds number. This model tends indeed to produce an excessive amount of turbulent eddy viscosity on this kind of flows [24]. For this reason, it represents an optimal baseline for testing the field inversion approach and evaluating how much the original model can be improved.

The mass-averaged RANS equations are reported in the following:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \quad (2)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u}(E + p)) = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u} - \mathbf{q}), \quad (3)$$

$$\frac{\partial \rho \hat{\nu}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \hat{\nu}) = \rho(P - D) + \frac{1}{\sigma} \nabla \cdot (\rho(\nu + \hat{\nu}) \nabla \hat{\nu}) + \frac{c_{b2}}{\sigma} \rho (\nabla \hat{\nu})^2 - \frac{1}{\sigma} (\nu + \hat{\nu}) \nabla \rho \cdot \nabla \hat{\nu}, \quad (4)$$

where ρ , \mathbf{u} , p , E , ν , $\hat{\nu}$, \mathbf{x} and t are density, velocity, pressure, total energy per unit volume, molecular viscosity, modified eddy viscosity, spatial position and time, respectively. A fluid with constant specific heat ratio γ and constant viscosity is considered. The following equation for the energy is considered:

$$E = \frac{P}{\gamma - 1} + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u}, \quad (5)$$

where γ is the specific heat ratio. The viscous stress tensor $\boldsymbol{\tau}$ includes both the molecular and eddy viscosity contributions and its components are given by:

$$\tau_{ij} = 2\rho(\nu + \hat{\nu} f_{v1}) \left(\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right). \quad (6)$$

The production P and destruction D terms in Eq. 4 are computed as follows:

$$P = c_{b1} \tilde{S} \tilde{\nu}, \quad D = c_{w1} f_w \left(\frac{\tilde{\nu}}{d} \right)^2, \quad (7)$$

with the following definitions:

$$f_w = g \left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right)^{1/6}, \quad g = r + c_{w2}(r^6 - r), \quad r = \min \left(\frac{\tilde{\nu}}{\tilde{S}^2 \kappa^2 d^2}, r_{lim} \right), \quad (8)$$

$$\tilde{S} = \begin{cases} S + \bar{S} & \text{if } \bar{S} \geq -c_{v2} S, \\ S + \frac{S(c_{v2}^2 S + c_{v3} \bar{S})}{(c_{v3} - 2c_{v2})S - \bar{S}} & \text{if } \bar{S} < -c_{v2} S, \end{cases} \quad (9)$$

where S is the vorticity magnitude and \bar{S} is:

$$\bar{S} = \frac{\tilde{\nu}}{\kappa^2 d^2} f_{v2}. \quad (10)$$

The functions f_{v1} and f_{v2} depend on the viscosity ratio $\chi = \frac{\tilde{\nu}}{\nu}$:

$$f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}. \quad (11)$$

110 The constants σ , c_{b1} , c_{b2} , c_{v1} , c_{w1} are defined in [23]. The last three terms
 111 which appear in Eq. 4 represent conservative diffusion, non-conservative
 112 diffusion and cross-diffusion. This last term comes from the combination of
 113 the original SA equation with the mass conservation equation, following [23].

114 Finally, the heat flux \mathbf{q} is described by the Fourier's law:

$$\mathbf{q} = - \left(\frac{c_p \mu}{Pr} + \frac{c_p \rho \hat{\nu} f_{v1}}{Pr_t} \right) \nabla T, \quad (12)$$

115 where T , c_p , Pr and Pr_t are the temperature, the constant pressure specific
 116 heat capacity, the Prandtl number and the turbulent Prandtl number. The
 117 test cases considered in this work refer to experiments performed with air
 118 and so the following values are assumed: $\gamma = 1.4$, $Pr = 0.72$ and $Pr_t = 0.9$.

119 3. Implicit Discontinuous Galerkin discretization

120 The discontinuous Galerkin (DG) scheme is used in this work for the
 121 spatial discretisation on the governing equations. This approach is charac-
 122 terised by a significant flexibility since it allows to easily manage high-order
 123 reconstructions on unstructured meshes. The main idea behind this kind
 124 of scheme consists in adopting a high-order polynomial reconstruction in-
 125 side each element without any continuity constraint at the interface between
 126 different elements. As a result, the scheme can be easily exploited in the
 127 framework of automatic adaptive approaches, in which both the size (h-
 128 adaptivity, [25, 26, 27, 28]), the order (p-adaptivity [29, 30, 31]) or both
 129 properties (hp-adaptivity, [32, 33, 34]) can be locally adapted following some
 130 error indicators.

131 The computational domain Ω is discretised with a hybrid mesh which
 132 contains a structured boundary layer mesh close to the body surrounded by
 133 an unstructured mesh. The grid is generated by means of Gmsh [35] with the
 134 Frontal-Delaunay for Quads algorithm. The management of the unstructured
 135 grid in the parallel MPI environment is performed through the DMPlex class
 136 [36] provided by the PETSc library [37].

137 The numerical approximation of the l -th conservative variable $u_l(\mathbf{x}, t)$
 138 inside each element Ω_e is described by a modal basis with size $N_e = \frac{(k+1)(k+2)}{2}$
 139 with a reconstruction order k :

$$u_l(\mathbf{x}, t) = \sum_{i=1}^{N_e} \tilde{u}_{li}(t) \phi_i(\mathbf{x}) \quad 1 \leq i \leq N_e, \quad (13)$$

140 where $\tilde{u}_{li}(t) \in \mathbb{R}^{N_e}$ contains the degrees of freedom inside the element for
 141 the l -th conservative variable. The basis functions $\phi_i(\mathbf{x})$ are obtained by the
 142 modified Gram-Schmidt orthonormalisation applied to a set of monomials de-
 143 fined in the physical space, following the approach of Bassi et al. [38]. In this
 144 work a third order accurate DG scheme is used ($k = 2$, $N_e = 6$). The spatial
 145 discretisation is completed by a projection of the governing equation on the
 146 space of the approximation functions. The resulting weak formulation con-
 147 sists of a set of ordinary differential equations in time. The convective terms
 148 which appear in the numerical fluxes at the interface between the elements
 149 are evaluated by means of an approximate Riemann problem solver (follow-
 150 ing [39] and [40]). Diffusive terms are evaluated by means of a recovery-based
 151 approach [41].

152 Time integration is performed here by means of the linearised implicit
 153 Euler method. Since steady problems are considered the use of a first order
 154 time integrator is deemed suitable since it does not influence the accuracy
 155 of the final steady solution and it has good dissipative properties which are
 156 useful to accelerate the numerical transients. The solution of the linear sys-
 157 tem which is obtained at each time step is performed in parallel by means of
 158 the GMRES algorithm with the additive Schwarz preconditioner provided by
 159 the PETSc library [37]. The GMRES algorithm is employed by setting the
 160 maximum number of iterations to 200, the dimension of the Krylov subspace
 161 to 100 and the absolute tolerance to 10^{-12} . The CFL number which controls
 162 the time step size is automatically adjusted according to the evolution of the
 163 residuals following the pseudo-transient continuation strategy [42]. In par-
 164 ticular, the CFL number is allowed to vary between 10^2 and 10^4 . During the
 165 first steps of the transient, a feedback filtering procedure [43] is applied to
 166 remove potential instabilities which can appear due to the large CFL num-
 167 ber. This filtering procedure is deactivated when the residuals drop under a
 168 certain threshold and so it does not influence the steady solution.

169 4. Field inversion and machine learning in a DG framework

170 The field inversion approach proposed by [14] requires to define a goal
 171 function G which measures the distance between the experimental data and
 172 the predicted numerical results. The procedure requires the solution of an
 173 optimisation problem in which a field $\beta(x)$ is found in order to minimise
 174 the goal function G . The field $\beta(x)$ is then introduced in a correction term
 175 $h(\beta(x))$ which multiplies the production term in the SA transport equation:

$$\frac{\partial \rho \hat{v}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \hat{v}) = \rho [h(\beta)P - D] + \frac{1}{\sigma} \nabla \cdot (\rho(\nu + \hat{v}) \nabla \hat{v}) + \frac{c_{b2}}{\sigma} \rho (\nabla \hat{v})^2 - \frac{1}{\sigma} (\nu + \hat{v}) \nabla \rho \cdot \nabla \hat{v}. \quad (14)$$

176 In the original works of [14, 44] the correction was chosen as $h(\beta) = \beta$. In this
 177 work, different choices are investigated for the function $h(\beta)$, as described in
 178 the next section.

179 As far as the goal function G is concerned, the following choice is made:

$$G = \int_w (M_s - M_s^{exp})^2 dl + \lambda \int_{\Omega} (\beta - 1)^2 d\Omega. \quad (15)$$

180 The first term is a line integral performed on the wall of the blade and allows
 181 to evaluate the norm-2 error on the wall isentropic Mach number distribution
 182 M_s , which is defined as:

$$M_s = \sqrt{\frac{2}{\gamma - 1} [(p_i^0 / p_w)^{(\gamma - 1)/\gamma} - 1]}, \quad (16)$$

183 where p_w is the static pressure at wall and p_i^0 is the inlet total pressure.
 184 The second term is an area integral on the computational domain Ω which
 185 acts as a Tikhonov regularisation [45]: it penalises the goal function when the
 186 correction factor is far from 1. This is useful to avoid unnecessary corrections
 187 which could be introduced during the optimisation process but which are not
 188 required in the final optimal solution. The choice of the penalisation constant
 189 λ will be discussed in the next Section.

190 In order to solve the optimisation problem, a simple gradient descent
 191 method is applied. The field β will be described in terms of the same basis
 192 functions used for the conservative variables. Starting from the original SA
 193 model ($h(\beta(x)) = 1$) the degrees of freedom related to the field β are updated
 194 with the gradient descent method:

$$\tilde{\beta} = \tilde{\beta} - \delta \frac{dG}{d\tilde{\beta}}, \quad (17)$$

195 where δ is the step size that in this work is chosen constant for simplicity
 196 ($\delta = 0.1$). Since the dimension of the optimisation problem is related to
 197 the total number of degrees of freedom per equation the computation of
 198 the gradient $\frac{dG}{d\tilde{\beta}}$ by means of numerical differentiation would be prohibitive.

199 For this reason, an adjoint-based gradient evaluation was implemented. The
 200 gradient of the goal function G with respect to the degrees of freedom of
 201 the field $\beta(x)$ is computed as:

$$\frac{dG}{d\tilde{\beta}} = \frac{\partial G}{\partial \tilde{\beta}} + \psi^T \frac{\partial R}{\partial \tilde{\beta}}, \quad (18)$$

202 where R represents the residual of the governing equations. The first term
 203 contains only the contributions related to the penalisation integral which
 204 appears in the goal function. The adjoint variable Ψ is computed by the
 205 solution of the following linear system with the GMRES iterative solver:

$$\left[\frac{\partial R}{\partial \tilde{u}} \right]^T \Psi = - \left[\frac{\partial G}{\partial \tilde{u}} \right]^T, \quad (19)$$

206 in which the jacobian matrix $\left[\frac{\partial R}{\partial \tilde{u}} \right]$ is already available from the implicit time
 207 integrator and the term $\left[\frac{\partial G}{\partial \tilde{u}} \right]$ contains the derivatives of the goal function
 208 with respect to the fluid dynamics degrees of freedom. This last term was
 209 computed by means of automatic differentiation with the Tapenade tool [46].
 210 Summarising, the procedure works as follows. First of all, a steady solution
 211 with the original SA model is obtained. The solution is considered steady
 212 when the residuals of all the governing equations are lower than 10^{-6} . Usua-
 213 ally, the SA equation is the one which converges with the lowest speed so
 214 when the condition is satisfied the residuals of the Eqs. 1-3 are orders of
 215 magnitudes lower (typically around 10^{-8} - 10^{-10}). When the steady solution
 216 is reached, the gradient $\frac{dG}{d\tilde{\beta}}$ is computed by the adjoint approach and the
 217 correction field is updated. This generates a transient which is solved in
 218 time up to a new steady solution. Since the perturbation introduced by the
 219 correction update is small, the transient can be easily solved by marching in
 220 time with a very large CFL number. For example, in this work the constant
 221 value CFL=5000 is used for this part of the computation. The procedure is
 222 repeated until the goal function does not show any significant improvement.

223 The correction field $h(\beta(x))$ obtained by the inversion process can be
 224 exploited for different purposes. On one hand, it gives insight for the devel-
 225 opment of new turbulence models since it shows where and how the original
 226 model fails. On the other hand, it is possible to directly generalise the cor-
 227 rection in order to obtain a new model which can be used for predictive
 228 simulations. For example, Duraisamy and Durbin [47] used the results of
 229 field inversion to define a transport equation for an intermittency factor,

230 where the different terms of the transport equation are computed by means
 231 of machine learning techniques. Alternatively, it is possible to find a local
 232 closure which allows to define the correction field as a function of local phys-
 233 ical quantities [14, 44]. This last approach is followed in the present work.
 234 In particular, the results of the inverse problem will be exploited to train
 235 an Artificial Neural Network (ANN) which can then be used to define an
 236 augmented version of the SA model.

237 5. Field inversion on the T106c cascade

238 The field inversion approach is applied here to the flow around the T106c
 239 gas turbine cascade. This profile is representative of high-lift low pressure
 240 gas turbines in modern turbofan engines. The cascade was experimentally
 241 investigated at the VKI and some experimental results are available from
 242 the literature [48, 49, 50]. In particular, the wall isentropic Mach number
 243 distribution, the mass averaged kinetic losses and exit angle in the wake are
 244 available for several values of the Reynolds number. The flow field is studied
 245 for an inlet angle $\alpha = 32.7^\circ$, an isentropic exit Mach number $M_{2s} = 0.65$
 246 and different values of the exit isentropic Reynolds number $8 \cdot 10^4 \leq Re_{2s} \leq$
 247 $2.5 \cdot 10^5$. The Reynolds number Re_{2s} is defined by using the blade chord and
 248 the isentropic exit velocity and density. The dynamic viscosity is assumed
 249 constant. The turbulence intensity during the experiments was very low
 250 (0.9%): for this reason all the RANS simulations are performed by setting a
 251 very small value of inlet eddy viscosity ($\tilde{\nu}/\nu = 0.1$).

252 Houmorziadis [51] showed that the Reynolds number in low pressure gas
 253 turbines of turbofan engines is the range between $10^5 - 4 \cdot 10^5$ where the
 254 smaller values are observed in cruise conditions and the higher values are
 255 obtained at take-off. The high-lift profiles can show large laminar separations
 256 at low values of Reynolds number. When the Reynolds number is increased
 257 the separation transforms from an open separation to a closed separation in
 258 which there is a separation bubble followed by reattached flow. The evolution
 259 from one configuration to the other takes place in a small range of Reynolds
 260 number and so the flow is quite sensitive to the working condition. The
 261 presence of separation can be easily noticed in the experimental studies on
 262 these flows by checking the wall isentropic Mach number distribution: the
 263 separation is usually related to the presence of a plateau in the distribution.
 264 Singh et al.[44] showed that the wall pressure distribution (which is directly
 265 related to the isentropic Mach number distribution) can be effectively used

266 in the field inversion approach for improving the prediction of separated
 267 flows. They indeed showed that the field inversion based on the wall pressure
 268 distribution can significantly improve the prediction of the Reynolds stresses
 269 in the separation region [44]. For these reasons, the field inversion algorithm
 270 used in this work will use the error on the wall isentropic Mach number
 271 distribution as goal function.

272 First of all, a convergence study is performed on the T106c cascade with
 273 the original SA model at the highest Reynolds number ($Re_{2s} = 2.5 \cdot 10^5$).
 274 Three different meshes and two reconstruction orders ($1 \leq k \leq 2$) are evalu-
 275 ated. The convergence level is assessed by checking the mass averaged value
 276 of the kinetic losses in a control section located $0.465c_x$ behind the trailing
 277 edge. The kinetic losses are defined in the following way:

$$\zeta = 1 - \frac{1 - (p_e/p_e^0)^{(\gamma-1)/\gamma}}{1 - (p_e/p_i^0)^{(\gamma-1)/\gamma}}, \quad (20)$$

278 where p_e , p_e^0 and p_i^0 are the static pressure in the control section, the total
 279 pressure in the control section and the inlet total pressure, respectively. The
 280 results of the convergence analysis are reported in Table 1 which shows the
 281 number of elements n_{ele} , the number of degrees of freedom per equation
 282 n_{DOF} and the predicted averaged losses. It is useful to remember that in the
 283 asymptotic range mesh refinement gives a fixed convergence order (depending
 284 on k) while order refinement gives exponential convergence.

285 We emphasise that the losses in the wake represent a better goal func-
 286 tion for the convergence assessment with respect to the wall isentropic Mach
 287 number distribution because the original SA model over-predicts significantly
 288 the turbulence eddy viscosity and so it gives a wall isentropic Mach number
 289 distribution which is very similar to what would be obtained by an inviscid
 290 Euler simulation, regardless of the mesh resolution. In contrast, the wake
 291 losses are influenced by the mesh resolution in the boundary layer and in the
 292 wake region. The mesh C reported in Tab.1 will be used for all the follow-
 293 ing simulations with a third order accurate DG scheme ($k = 2$). The mesh
 294 contains 40436 elements and so the total number of degrees of freedom per
 295 equation is equal to 242616. The dimensionless wall cell size is $y^+ < 1$ on
 296 the entire surface.

297 As reported in Equation 14, the field inversion approach requires to alter
 298 the production term by the presence of the correction factor $h(\beta)$. In this
 299 work, different expressions for $h(\beta)$ are investigated. The most straightfor-
 300 ward approach, which was used by Singh et al. [44] for the study of wind

	n_{ele}	n_{DOF}	ζ
Mesh A, k=1	11480	34440	2.39E-002
Mesh B, k=1	21195	63585	2.27E-002
Mesh C, k=1	40436	121308	2.24E-002
Mesh A, k=2	11480	68880	2.25E-002
Mesh B, k=2	21195	127170	2.24E-002
Mesh C, k=2	40436	242616	2.24E-002

Table 1: Mass averaged kinetic losses: convergence with grid size and reconstruction order

301 turbine airfoils, consists in setting :

$$h(\beta) = \beta \quad \beta \in \mathbb{R}. \quad (21)$$

302 In this way the correction factor is free to assume both positive and negative
303 values and so the correction term is very general. However, this generality
304 comes with a price: since $h(\beta)$ is not limited it can lead to unstable numerical
305 results during the transients which must be solved in predictive simulations.
306 An alternative approach, experimented in this work, consists in setting

$$h(\beta) = \beta^2 \quad \beta \in \mathbb{R}. \quad (22)$$

307 In this way the correction term is not allowed to assume negative values. This
308 means that the generality of the approach is reduced but the robustness of
309 the simulation is increased because the correction term cannot change the
310 nature of the production term (it can, in the limit, set the production to zero
311 but it cannot transform the production term into a destruction term).

312 A third approach, which showed the most robust results in this work,
313 is reported in the following. The idea behind this approach is to mimic
314 the behaviour of intermittency models in which the production term of the
315 RANS model is reduced by a factor defined in the range $[0, 1]$ in order to
316 reproduce transition phenomena. Following this approach, the correction
317 term is defined as a smooth ramp function of β :

$$h(\beta) = \begin{cases} 0 & \text{if } \beta \leq 0, \\ 3\beta^2 - 2\beta^3 & \text{if } 0 < \beta < 1, \\ 1 & \text{if } \beta \geq 1. \end{cases} \quad (23)$$

318 This last approach is the least general between the three alternatives exam-
 319 ined in this work but it is the most robust. This is due to the fact that,
 320 in the end, the correction factor h will be expressed by means of an ANN.
 321 When the SA model augmented by the ANN correction term will be used for
 322 actual predictions, the ANN will be asked to compute the correction factor
 323 for input values which could be outside of the range explored in the train-
 324 ing database. This is very likely to happen during the numerical transient
 325 which must be solved before getting the steady solution. However, ANNs
 326 are known for their poor extrapolation accuracy and so the use of a more
 327 general expression (like for example the one defined by Equation 21) would
 328 allow the presence of unlimited values of the correction factor. In contrast,
 329 when the correction factor is limited in the range $0 \leq h \leq 1$ the model can
 330 behave, in the limit, as the original SA model (when $h \rightarrow 1$) or as the laminar
 331 Navier-Stokes equations (when $h \rightarrow 0$).

332 In order to understand whether the limitation introduced by Equation 23
 333 affects the ability of the field inversion to match the experimental data, the
 334 different definitions of $h(\beta)$ are tested on the T106c cascade. In particular,
 335 the gradient based optimisation process is carried out for the T106c at $Re_{2s} =$
 336 $8 \cdot 10^4$ and $Re_{2s} = 2.5 \cdot 10^5$. The plot in Figure 1 shows the history of
 337 the goal function during the optimisation process. The results shows that
 338 after approximately 50 steps of the gradient descent algorithm a minimum
 339 is reached. This optimisation is carried out by starting from the original SA
 340 model with $h = 1$ in all the domain and using the unlimited correction factor
 341 defined by Eq. 21 with $\lambda = 0$.

342 The optimal field obtained from this first step is then used as initial field
 343 for a second optimisation in which the correction factor is limited according
 344 to Eq. 23. It is useful to emphasise that, in order to apply the correction
 345 factor defined by Eq. 23, it is not possible to start with a uniform field with
 346 $\beta = 1$. This is due to the fact that the derivative of the smooth ramp function
 347 is null for $\beta = 1$ and so it would not be possible to update the solution since
 348 the gradient of the goal function would remain to zero according to Eq. 18
 349 ($\frac{\partial R}{\partial \beta} = \frac{\partial R}{\partial g} \frac{\partial g}{\partial \beta}$, with $\frac{\partial g}{\partial \beta} = 0$ for $\beta = 1$). In order to compare the two approaches,
 350 the wall isentropic Mach number distribution is reported in Figure 2 for the
 351 original SA model and the optimised solutions related to Eq. 21 and 23. The
 352 results for the correction factor defined by Eq.22 are not reported in the plot
 353 since they overlap the other results related to 21 and 23. The figure shows
 354 also the available experimental data which are used to drive the optimisation

process. The optimal solutions show a good match with the experimental data and a significant improvement with respect to the baseline model. This test confirms that the limited correction factor defined by Eq. 23 is able to provide an optimal solution which is comparable to the results provided by the unlimited correction factor. This is due to the fact that the original SA model overestimates significantly the turbulence production in this kind of flows and so the use of a correction factor limited between 0 and 1 is sufficient to correct the model. In this sense, the correction factor proposed in this work acts exactly as a intermittency correction in the framework of laminar-to-turbulence transition. After this analysis, the limited correction factor defined by Eq. 23 was chosen for all the following simulations. The plots in Figure 3 show the Mach field for the original SA model and optimal model at $Re_{2s} = 8 \cdot 10^4$ and $Re_{2s} = 2.5 \cdot 10^5$. The optimal solution at $Re_{2s} = 8 \cdot 10^4$ is characterised by a large open separation which is completely missed by the original SA model. The optimal solution at $Re_{2s} = 2.5 \cdot 10^5$ shows a small separation bubble followed by reattachment. Again, this separation is missed by the original SA model.

Finally, the correction field at $Re_{2s} = 8 \cdot 10^4$ and $Re_{2s} = 2.5 \cdot 10^5$ for the case defined by Eq. 23 is reported in Figures 4 and 5 for $\lambda = 0$ and $\lambda = 10^{-3}$, respectively. An analysis of the pictures shows clearly that the adjoint approach obtained an optimal solution in which the production term is deactivated in the boundary layer for the first portion of the suction side: the algorithm has recovered a laminar separation just by using the knowledge on the experimental wall isentropic Mach number distribution. As far as the influence of λ is concerned, a study with $\lambda = 0, 10^{-2}, 10^{-3}, 10^{-4}$ is performed. These values are chosen by running a preliminary simulation with $\lambda = 0$ and then evaluating the order of magnitude of the two integrals which appear in the goal function defined by Eq. 15. For all these values, the optimal wall isentropic Mach number distribution does not show significant variations. The weak influence of the parameter λ can be seen in Figures 4 and 5 where the higher value of λ tends to avoid unnecessary corrections at the end of the separation region. All the results reported in the following refer to the value $\lambda = 10^{-3}$.

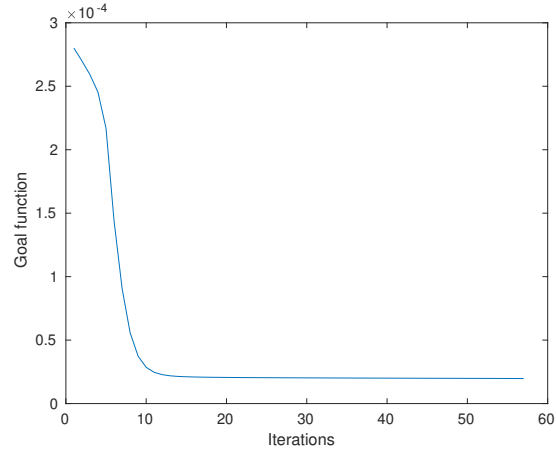


Figure 1: Adjoint-based optimization history for T106c at $Re_{2s} = 8 \cdot 10^4$ with $\beta \in R$

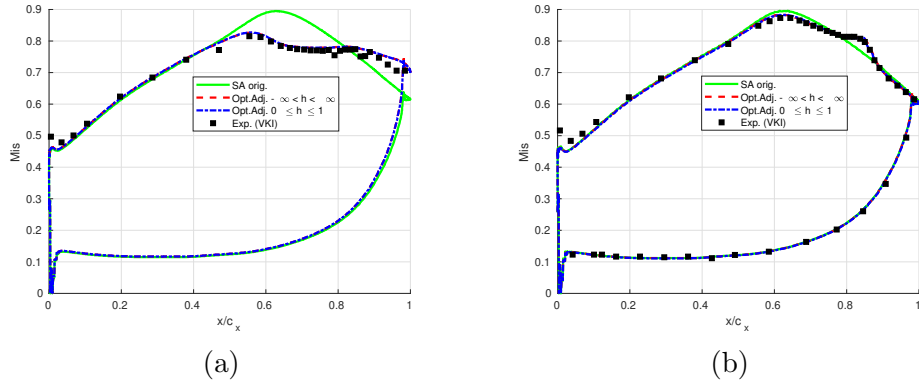


Figure 2: Comparison between original SA model, optimized model and experimental results in terms of Mis distribution for the T106c at $Re_{2s} = 8 \cdot 10^4$ (a) and $Re_{2s} = 2.5 \cdot 10^5$ (b)

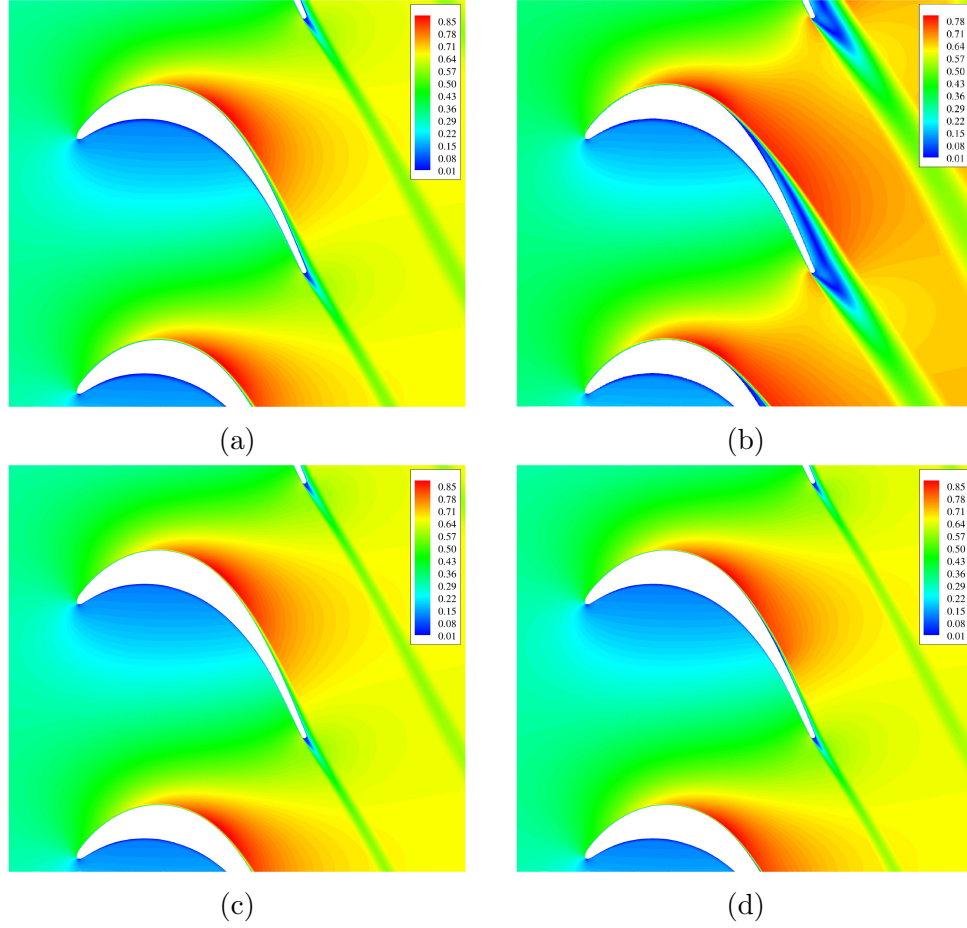


Figure 3: Mach field for T106c with the original SA model (a,c) and with optimised model (b,d) at $Re_{2s} = 8 \cdot 10^4$ (a,b) $Re_{2s} = 2.5 \cdot 10^5$ (c,d)

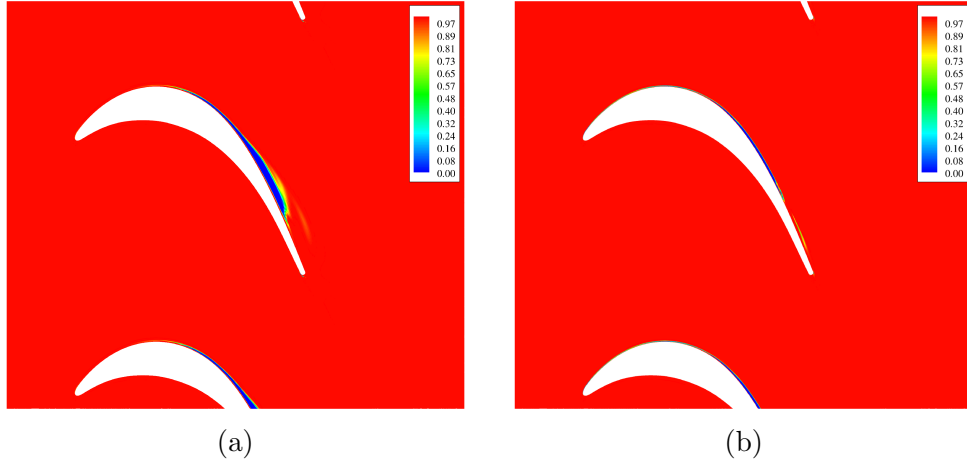


Figure 4: Correction field $h(x)$ for T106c at $Re_{2s} = 8 \cdot 10^4$ (a) and $Re_{2s} = 2.5 \cdot 10^5$ (b) with $\lambda = 0$

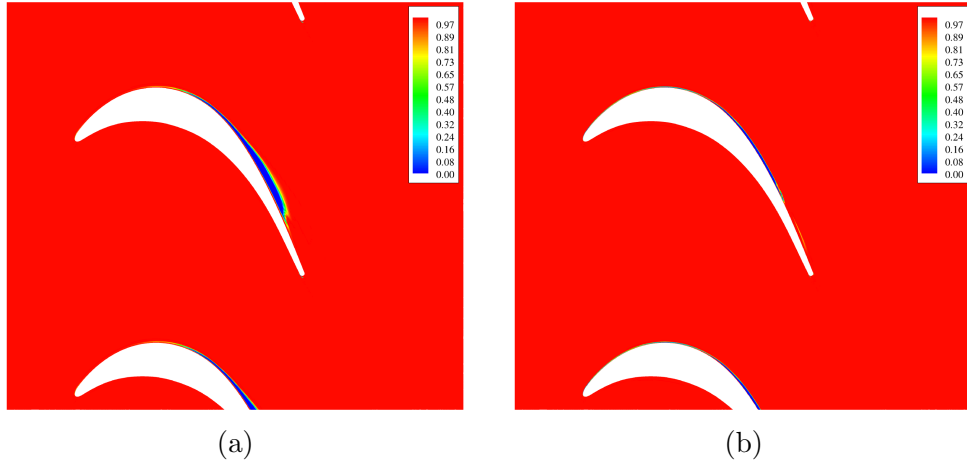


Figure 5: Correction field $h(x)$ for T106c at $Re_{2s} = 8 \cdot 10^4$ (a) and $Re_{2s} = 2.5 \cdot 10^5$ (b) with $\lambda = 10^{-3}$

389 6. Machine learning on the T106c cascade

390 The field inversion algorithm described in the previous section is able to
391 provide a correction field which alters the original SA model in order to match
392 very well the experimental results for two different working conditions. In
393 this section this result will be generalised in order to express the correction
394 factor as a function of some physical features. In particular, several choices
395 related to the inputs and the architecture of the ANN used to express the
396 correction factor will be investigated.

397 6.1. Choice of the inputs

398 The choice of the input variables of the ANN is not a trivial task because
399 it is not possible to know a-priori whether the chosen inputs determine univo-
400 cally the output. Furthermore, it is necessary to avoid input variables which
401 would introduce a dependency on the particular frame of reference which
402 is used to study the problem (i.e. Galilean invariance must be satisfied).
403 Finally, there should not be strong correlations between the different input
404 variables and they should be chosen as adimensional quantities in order to
405 get general results. A natural choice is to identify some adimensional groups
406 which appear in the source term of the original RANS model and use them
407 as input for the ANN. This choice was for example carried out by Singh et
408 al. [44].

409 A similar approach is used in this work but particular attention is devoted
410 here to the robustness and the prediction ability of the model. The following
411 five input variables are used: χ , $\log(\tau/\tau_{ref} + \epsilon)$, f'_d , $\log(P/(D + \epsilon) + \epsilon)$ and
412 $\log(|\nabla \tilde{\nu}|d/(\nu + \tilde{\nu}) + \epsilon)$. The plots in Figure 6 show the distribution for all
413 the inputs variables in the optimised solution at $Re_{2s} = 8 \cdot 10^4$.

414 The first input, χ , simply represents the turbulent intensity. The quan-
415 tity τ/τ_{ref} is obtained by normalising the modulus of the stress tensor with
416 respect to a reference stress. The reference stress is defined here as $\tau_{ref} =$
417 $\rho(\nu + \tilde{\nu})^2/d^2$ which makes this input a local quantity. In contrast, Singh et al.
418 [44] used a non local normalisation in which the stress tensor is normalised
419 with respect to the wall stress τ_w . However, such non-local terms are avoided
420 in this work since the presence of non-local terms reduces significantly the
421 scalability of the discretisation in a parallel environment. Furthermore, the
422 physical meaning of using τ_w for the normalisation is clear for the mesh points
423 in the boundary layer but is not so clear for other regions, like for example
424 the wake. Finally, a logarithmic scaling of the quantity τ/τ_{ref} was observed

425 to significantly improve the fitting of the database. The additive constant
 426 $\epsilon = 10^{-5}$ is introduced to prevent the argument of the logarithm to become
 427 null.

428 The term f'_d is introduced in this work as a modification of the term f_d
 429 used by Singh et al. [44] and originally proposed by [52] in the framework of
 430 Detached Eddy Simulations. The terms are defined as:

$$f_d = 1 - \tanh((8r_d)^3), \quad f'_d = 1 - \tanh((r_d)^{0.5}), \quad (24)$$

431 where the quantity r_d is an adimensional group obtained by combining wall
 432 distance, turbulence and molecular viscosity and velocity gradient:

$$r_d = \frac{\nu + \tilde{\nu}}{d^2 \kappa^2 \sqrt{\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}}}, \quad (25)$$

433 where $\kappa = 0.41$ is the von Karman constant. The plot in Figure 6 explains
 434 why in this work the term f'_d is used instead of f_d : both terms are limited
 435 between 0 and 1 but f'_d allows to better describes the flow features close
 436 to wall while f_d tends to compress the information and does not allow to
 437 distinguish the different structures. This qualitative analysis was confirmed
 438 by a quantitative analysis which shows that an ANN with f'_d was able to
 439 better fit the database with respect to an equivalent ANN with f_d as input.

440 The term $\log(P/(D + \epsilon) + \epsilon)$ represents a convenient scaling of the ratio
 441 between the production P and destruction D terms of the SA model. In
 442 the work of Singh et al. [44] the ratio P/D is directly used while in this
 443 work a logarithmic scaling is used: this is due to the fact that the values
 444 assumed by this ratio are distributed in a wide range which covers several
 445 orders of magnitude and some numerical experiments confirmed that the
 446 fitting significantly improves with this scaling. Furthermore, both the nu-
 447 merator and the denominator of this quantity can go to zero in the presence
 448 of uniform fields or where the turbulence viscosity is zero and so the con-
 449 stant $\epsilon = 10^{-5}$ is introduced. Some numerical tests showed that the use of
 450 logarithmic scaling improves significantly the fitting of the database with the
 451 ANN. Finally, the adimensional gradient of the modified turbulent viscosity
 452 $\log(|\nabla \tilde{\nu}|d/(\nu + \tilde{\nu}) + \epsilon)$ is considered. This quantity was not used in [44] and
 453 does not appear in the production and destruction terms. However, it ap-
 454 pears in the cross production term (the last term of Eq. 4) and allows to
 455 identify regions with strong variations in the eddy viscosity. It is normalised

456 with respect to the wall distance and the sum of kinematic and eddy vis-
 457 cosity: this means that this quantity remains well conditioned even when
 458 the eddy viscosity tends to zero since the kinematic viscosity prevents the
 459 denominator to become zero. Even for this variable the logarithmic scaling
 460 was found to be useful to improve the fitting.

462 6.2. Choice of the ANN architecture

463 After choosing the input features, it is necessary to define the architecture
 464 of the ANN. In this work, feedforward ANNs are considered. As far as
 465 the activation functions are concerned, a common choice consists in using
 466 sigmoid functions for the hidden layers and linear functions for the output
 467 layer. However, since the chosen correction factor h is limited in the range
 468 $[0, 1]$ a sigmoid activation function is adopted also for the output layer: in
 469 this way the output of the ANN will be automatically limited in the range
 470 $[0, 1]$.

471 Particular care should be taken in choosing the number of hidden layers
 472 n_{HL} and the number of neurons per layer n_N . In particular it is necessary to
 473 find a compromise between the complexity of the network (which allows to
 474 capture the correlations hidden in the database) and its ability to perform
 475 predictions outside of the database. When the complexity of the network is
 476 increased its ability to reproduce the training database is enhanced because it
 477 has more degrees of freedom which can be adjusted to fit the data. However,
 478 if too many degrees of freedom are introduced the overfitting phenomenon
 479 can be observed: in this case the network behaves poorly during predictions
 480 because when the ANN has too many degrees of freedom the output shows
 481 strong oscillations for the points in the parameter space which do not exactly
 482 match a training point.

483 In order to find a suitable network by using a general criterion the fol-
 484 lowing approach is used. First of all, different architectures are considered
 485 ($1 \leq n_{HL} \leq 2$ $5 \leq n_N \leq 40$) and the ability of the networks to fit the
 486 database is investigated. Each network is trained in Matlab by means of
 487 the Levenberg-Marquadt algorithm with a goal function based on the mean
 488 squared error. The training is performed by dividing randomly the database
 489 in 3 subsets: one for training (70% of the data), one for validation (15% of
 490 the data) and one for test (15% of the data). The training set is actually
 491 used for the computation of the mean square error and for driving the train-
 492 ing process. The validation set is used during the training to verify that the

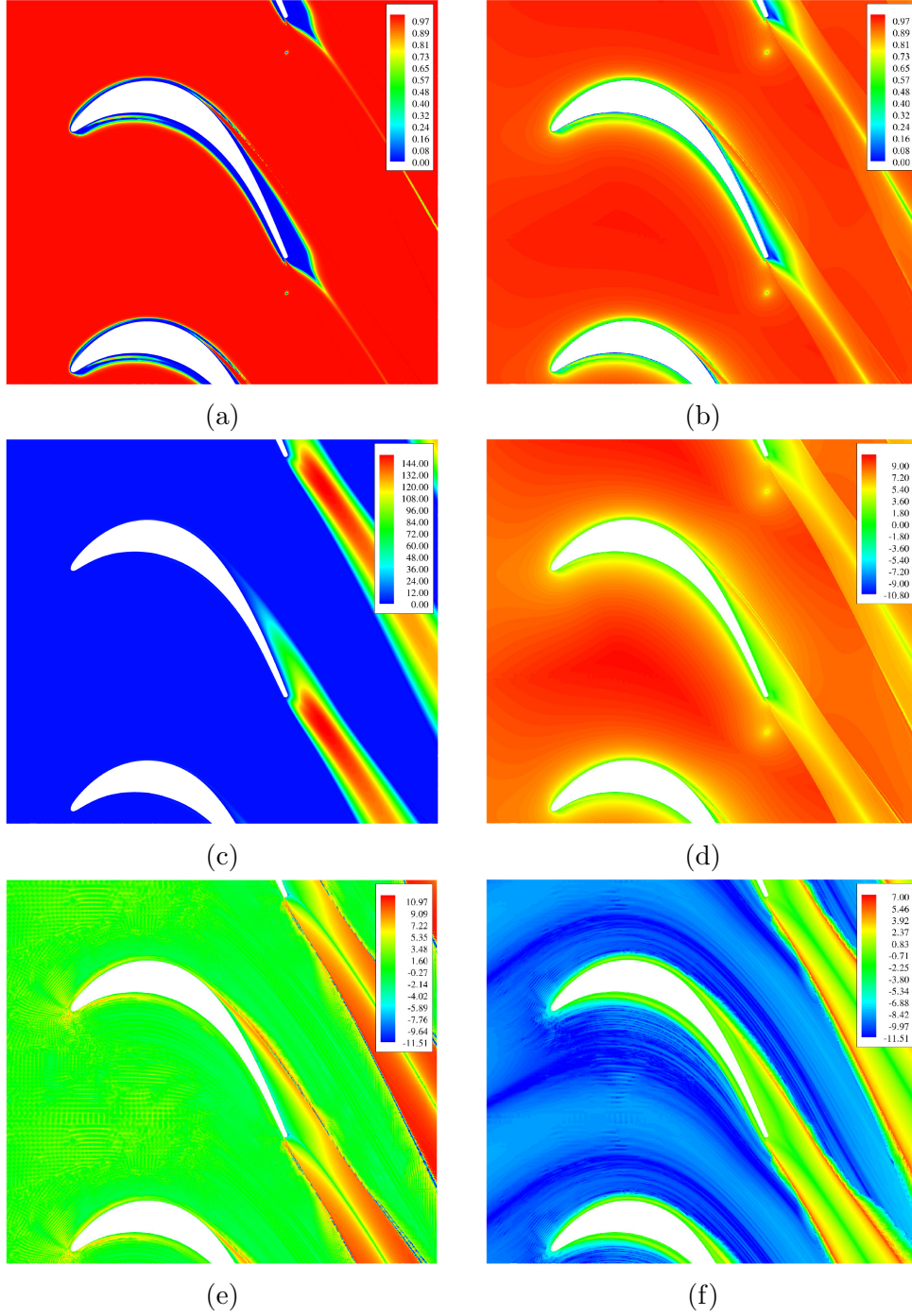


Figure 6: Input features for the neural network: f_d (a), f'_d (b), χ (c), $\log(\tau/\tau_{ref} + \epsilon)$ (d), $\log(P/(D + \epsilon) + \epsilon)$ (e), $\log(|\nabla \tilde{v}|d/(\nu + \tilde{v}) + \epsilon)$ (f)

ANN is still able to give good predictions for points which do not belong to the training set: when the validation error tends to increase the training is arrested, even if the training error is still decreasing, in order to limit the problem of overfitting. Finally, the test set is used to monitor the behaviour of the ANN on an external set of data which do not influence the training process (neither in the mean squared error computation nor in the validation checks for the overfitting). An example of training history is reported in Figure 7a in which it can be clearly seen that when the training is stopped the training error was still decreasing but the validation error just started to grow. In Figure 8 it is possible to see the regression plots for the different data sets: in each plot the abscissa represents the reference value in the database while the ordinate represents the approximated value computed by the network. The plots show also the fitting line which is compared with the ideal fitting line ($R=1$) which would be obtained if the ANN would be capable of perfectly fitting the data.

Another approach for avoiding overfitting was also investigated: Bayesian regularisation [53]. In Bayesian regularisation the mean square error goal function is augmented by a term which penalises large values of the weights. However, some experiments on the problems considered in this work showed that the splitting of the database in training, validation and test sets allows to achieve a better compromise between fitting and robustness with respect to the Bayesian regularisation.

A sequence of regression plots (on the test subset of the database) for the ANN 2×5 , 2×10 , 2×20 and 2×40 are reported in Figure 9: as the complexity of the network is increased its ability to reproduce the database is enhanced as can be clearly seen by the fact that the points tend to assume a distribution centered along the bisector of the quadrant. In Table 2 the regression coefficient R evaluated on the test subset of the database is reported for different ANN architectures.

	$n_N = 5$	$n_N = 10$	$n_N = 20$	$n_N = 40$
$n_{HL} = 1$	0.751	0.798	0.864	0.877
$n_{HL} = 2$	0.813	0.884	0.912	0.941

Table 2: Regression coefficient R for several architectures of the ANN (test subset of the database)

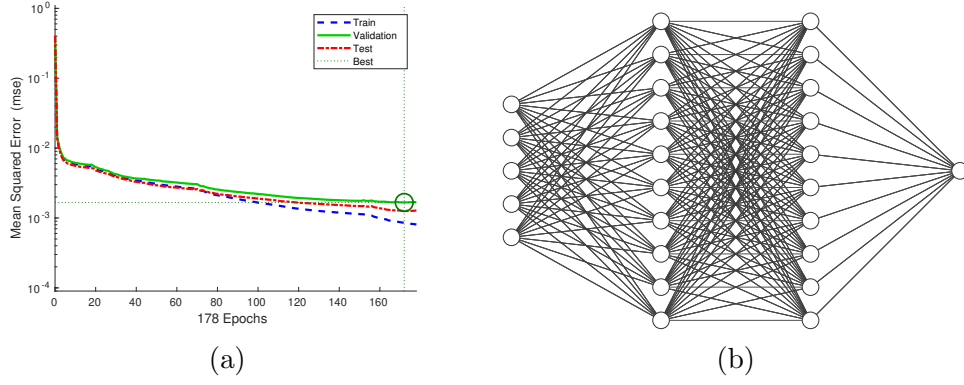


Figure 7: Training history (a) and architecture (b) for 2x10 ANN

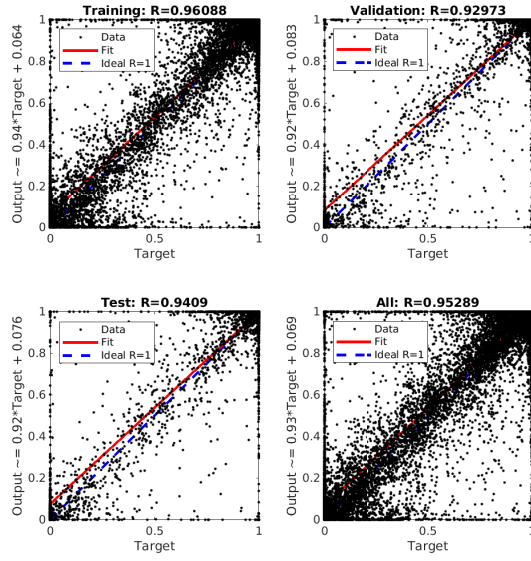
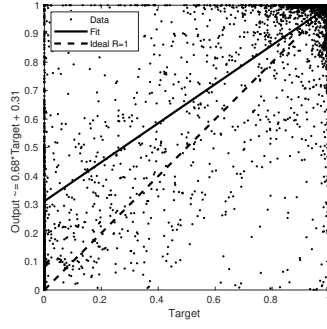
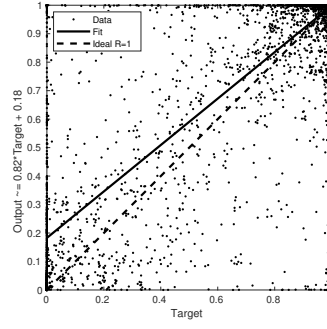


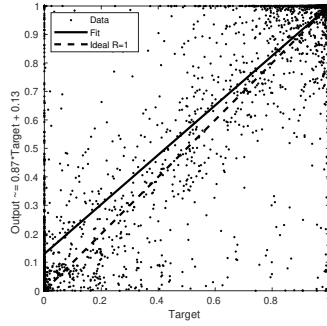
Figure 8: Training, validation and test error for 2x40 ANN



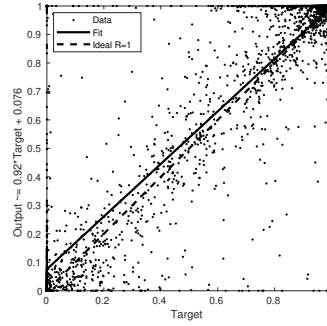
(a)



(b)



(c)



(d)

Figure 9: Regression plots for different ANN architectures on the test subset: 2x5 (a), 2x10 (b), 2x20 (c), 2x40 (d)

According to the previous analysis it would seem that the larger the network is, the better the result is. This is true for the fitting of the points in the database. However, it is fundamental to investigate the behaviour of the network coupled with the CFD solver for points which do not coincide exactly with the points in the database. In order to do this it is possible to run some CFD simulations at $Re_{2s} = 8 \cdot 10^4$ and $Re_{2s} = 2.5 \cdot 10^5$ with the correction term h estimated by the different ANNs. Apparently, this seems a useless check since the database used for the training is built from the optimal solution at these values of Reynolds number and so one could expect that the ANN should reproduce perfectly these working conditions. However, it is important to keep in mind that the regression coefficient R is always less than 1: this means that, even if the CFD simulation is initialised with the optimal solution obtained by the adjoint approach, the correction field reproduced by the ANN will not coincide exactly with the optimal one. As a consequence, the CFD solution will evolve towards a new steady solution. This introduces a perturbation in the input features given to the ANN: if the ANN is robust the new steady solution will be close to the optimal one. However, if the ANN is poorly conditioned because an excessive number of neurons has been chosen then the network will give a significantly different response. The experiments performed during this work suggested that the classical approach of splitting the database between training and validation sets does not guarantee the absence of overfitting when the ANN is coupled with the CFD solver: it seems that the coupling with the CFD solver introduces a sort of positive feedback which amplifies the overfitting problem.

In order to investigate this behaviour, some tests are performed by checking the wall isentropic Mach number distribution reported in Figure 10 for the ANNs with 2×5 , 2×10 , 2×20 and 2×40 neurons. It can be seen that the 2×5 network performs poorly because of its inability to reproduce the database. The networks with 2×10 and 2×20 neurons perform significantly better and give solutions which are very close to the optimal ones. The largest network with 2×40 neurons starts to show some problems at $Re_{2s} = 2.5 \cdot 10^5$ in which it is not able to reproduce the small separation bubble. According to this analysis, all the predictive simulations reported in the following will be performed by using the 2×20 ANN.

557

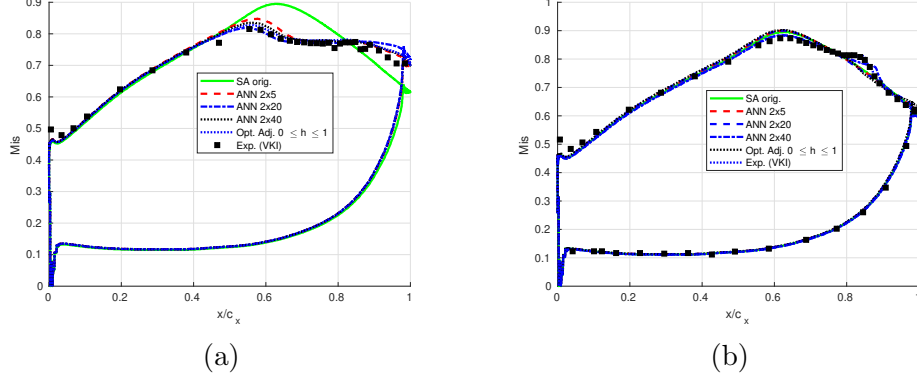


Figure 10: Comparison of different ANN architectures in terms of wall isentropic Mach number distribution on the T106c at $Re_{2s} = 8 \cdot 10^4$ (a) and $Re_{2s} = 2.5 \cdot 10^5$ (b):

7. Predictions

In the previous Section the procedure for choosing the architecture of the ANN is reported. Now, the chosen network is used to perform predictive simulation for working conditions and geometries which were not included in the database. As a first step all the simulations are performed by setting $h(x) = 1$, i.e. with the original SA model. Then the obtained steady solution is used to initialise a simulation in which the correction term is computed with the ANN. This approach speeds up the convergence since the ANN is not employed during the strong initial transient at the beginning of the simulation.

Furthermore, the numerical experiments showed that the robustness of the method during predictive simulations can be improved by limiting the input variables to the range used for the training. This is important because the ANN has been trained only on a few steady solutions and so during the transients which can appear in predictive simulations the input features could assume values which were not observed in the training database. In particular, if $h(\mathbf{Y})$ represents the ANN approximation of the correction factor and \mathbf{Y} is the vector of the five input variables, the modified expression $h(L(\mathbf{Y}))$ is used during predictive simulations, where the limiting function L is defined as:

$$L(Y_i) = \begin{cases} Y_i & \text{if } Y_i^{min} \leq Y_i \leq Y_i^{max}, \\ Y_i^{max} & \text{if } Y_i > Y_i^{max}, \\ Y_i^{min} & \text{if } Y_i < Y_i^{min}. \end{cases} \quad (26)$$

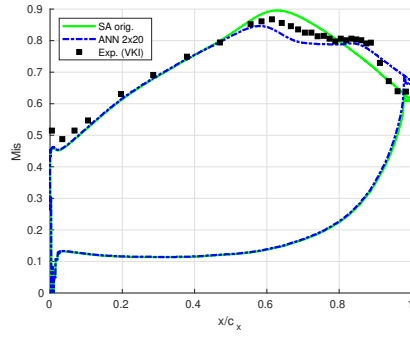
578 Here Y_i^{min} and Y_i^{max} represent the minimum and maximum values of the i -th
 579 input feature observed in the training database.

580 7.1. T106c cascade at different Reynolds number

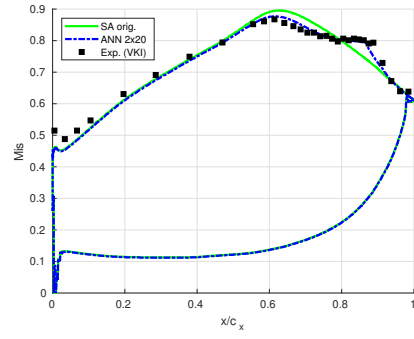
581 As a first test, the ANN augmented SA model is used to predict the flow
 582 field on the T106c at $Re_{2s} = 1.2 \cdot 10^5$, $1.6 \cdot 10^5$ and $2.1 \cdot 10^5$. In this range
 583 of Reynolds number a strong variation is observed in the solution due to the
 584 transition from open to closed separation. The results related to the wall
 585 isentropic Mach number distribution are reported in Figure 11 in which they
 586 are compared with the available experimental results and the original SA
 587 model. The experimental uncertainty on the wall isentropic Mach number
 588 ranged between 0.4 – 1.2% [48]. The ANN augmented SA model performs
 589 significantly better than the original model and the predictions are quite close
 590 to the experiment. Only the solution obtained at $Re_{2s} = 1.2 \cdot 10^5$ seems to
 591 overpredict the separation.

592 The results reported in Figure 11 refer to the M_{is} distribution used in the
 593 goal function which drove the field inversion and so it is natural to expect
 594 an improvement with respect to the original model. However, the prediction
 595 ability of the model was also investigated in terms of mass averaged kinetic
 596 losses ζ and exit angle β_2 in the wake, quantities which were not included
 597 in the goal function used for the optimisation. The average is performed in
 598 a control section located $0.465c_x$ behind the trailing edge, where c_x is the
 599 axial chord, in the same location used for the experimental measurements.
 600 The results of these tests are reported in Figure 12 which shows also the
 601 experimental results. The experimental uncertainty ranges between 10 – 20%
 602 [48]. As far as the losses are concerned, both the original SA model and the
 603 ANN augmented SA model perform well for high Reynolds number values:
 604 in particular, the results of the ANN augmented model are very close to
 605 the experimental data. However, for low Reynolds numbers the original SA
 606 model misses completely the separation and so it underpredicts significantly
 607 the losses. The ANN augmented SA model shows the correct trend and
 608 is quite close to the experimental results at $Re_{2s} = 8 \cdot 10^4$ (for which the
 609 optimisation was performed). However, the prediction at $Re_{2s} = 1.2 \cdot 10^5$
 610 overestimates the losses and so the curve with the ANN augmented results
 611 shows the wrong concavity with respect to the experimental results.

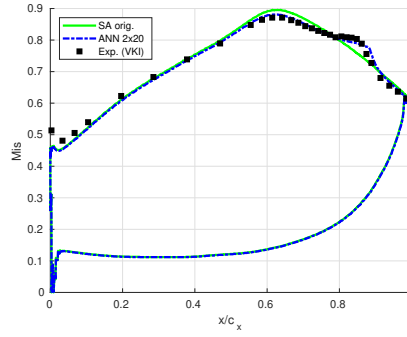
612 The plot shows also the results obtained by Benyahia et al. [54] with the
 613 SST- γ - Re_θ model based on the correlations proposed by [55], by Pacciani et
 614 al.[56] with the $k-\omega$ model coupled with a transport equation for the laminar



(a)



(b)



(c)

Figure 11: Wall isentropic Mach number distribution: predictions at $Re_{2s} = 1.2 \cdot 10^5$ (a), $Re_{2s} = 1.6 \cdot 10^5$ (b) and $Re_{2s} = 2.1 \cdot 10^5$ (c)

615 kinetic energy and by Babajee [50] with the SST- γ - Re_θ model [57, 58]. The
616 comparison shows a significant influence of the correlations which are used
617 to close the SST- γ - Re_θ model. The results obtained by Pacciani et al.[56]
618 are very close to the experimental data but their model is non-local because
619 it requires the computation of the vorticity thickness in the boundary layer:
620 this complicates the implementation of the model in a parallel environment
621 with unstructured meshes and requires particular care for the leading and
622 trailing edge regions.

623 The boundary condition for the turbulent kinetic energy equation which
624 appears in the SST model is clearly defined by the experimental inlet tur-
625 bulance intensity (0.9%). However, the SST model requires also an inlet
626 boundary condition for the ω equation which is usually prescribed by defin-
627 ing an inlet turbulence Reynolds number (Re_T). Babajee performed a study
628 on the choice of the inlet value for Re_T : in particular he found the optimal
629 value of Re_T which fits the experimental turbulence decay in the wind tunnel
630 without the cascade. However, when this value is imposed at the inlet, the
631 SST- γ - Re_θ model is not able to predict accurately the separation. For this
632 reason he performed a parametric study changing Re_T in order to match
633 at best the experimental results on the T106c. For this reason, the plot
634 shows two set of results related to the SST- γ - Re_θ model: the results with the
635 boundary condition which is coherent with the physical decay of turbulence
636 in the wind tunnel ($Re_T = TD$) and the results with an alternative value
637 which gives better predictions ($Re_T = 0.01$). As far as the average exit angle
638 is concerned, the ANN augmented SA model shows a better behaviour than
639 the original SA model at low Reynolds numbers while the two models give
640 similar results at higher Reynolds numbers. It is interesting to note that
641 the asymptotic value of the exit angle for high values of Reynolds number
642 presents an offset between experimental and numerical results. However,
643 this offset was observed also by other results in the literature as shown by
644 the SST- γ - Re_θ results from [50]. This discrepancy cannot be justified by
645 the experimental uncertainty which was estimated in the range $0.2 - 0.3$ de-
646 grees [48]. The excessively large separation predicted by the ANN augmented
647 model at $Re_{2s} = 1.2 \cdot 10^5$ leads to an overestimation of the exit angle for this
648 condition, similarly to what can be observed for the kinetic losses.

649

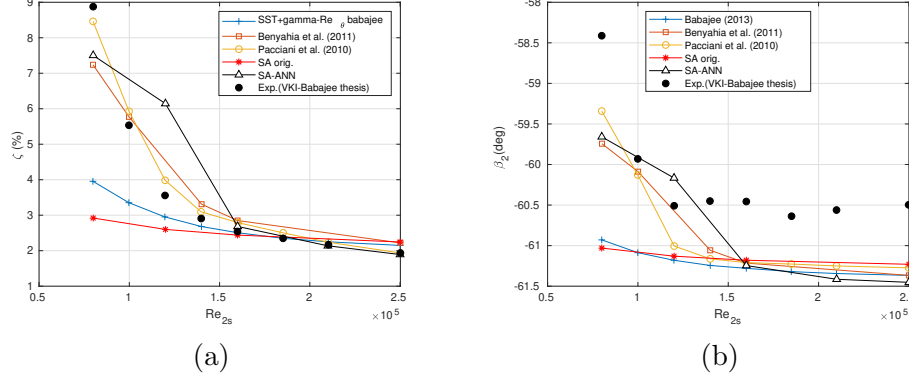


Figure 12: Average losses and exit angle for T106c cascade: comparison between original SA model, SA-ANN model and experimental results

7.2. T2 cascade

The prediction ability of the ANN augmented SA model is investigated also on another geometry, the T2 cascade. The simulations are carried out with a third order accurate DG scheme on a mesh with 59453 elements, corresponding to 356718 degrees of freedom per equation. The mesh resolution at the wall and in the wake region is the same used for the T106c, since both cascades are investigated at similar values of Reynolds number. The T2 airfoil was designed at the VKI for the same velocity triangles of the T106 (inlet angle $\alpha = 32.7^\circ$) but it is characterised by a larger pitch-to-chord ratio (1.05) and an increased diffusion rate along the rear suction side [50]. Also the Zweifel number is larger ($\Psi = 1.46$) with respect to the T106 ($\Psi = 1.24$). The isentropic exit Mach number is set to $M_{2s} = 0.65$. In Figure 13 and 14 the Mach number field at $Re_{2s} = 1.2 \cdot 10^5$ and $2.1 \cdot 10^5$ is reported for the original SA model and for the ANN augmented SA model. The plots show clearly the presence of a open separation at $Re_{2s} = 1.2 \cdot 10^5$ in the SA augmented results: the separation does not appear in the original SA results. The difference between the two models is less evident at the higher Reynolds number ($Re_{2s} = 2.1 \cdot 10^5$): a small separation region followed by reattachment is predicted by the SA augmented model while the original SA model does not show any sign of separation. In Figure 15 the predicted wall isentropic Mach number distribution is reported as a function of the curvilinear coordinate s along the blade surface, normalised with respect to the curvilinear length of the blade (s_0). The plots show also the experimental results in which the separation region can be identified by the presence of a plateau

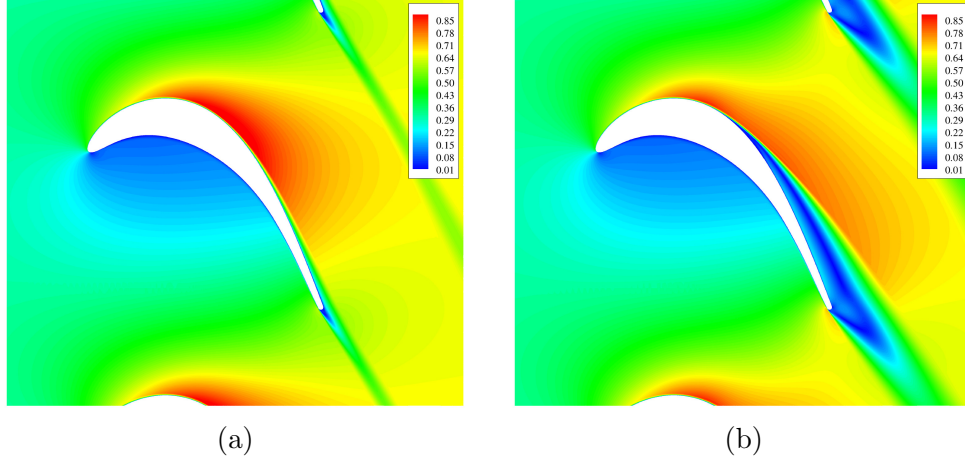


Figure 13: Mach field for the T2 cascade at $Re_{2s} = 1.2 \cdot 10^5$ with the original SA model (a) and with the ANN-SA model (b)

in the wall isentropic Mach number distribution. The ANN augmented SA model shows significant improvements with respect to the baseline SA model. As far as the comparison with the SST- γ - Re_θ results from [50] is concerned, at $Re_{2s} = 1.2 \cdot 10^5$ the ANN augmented SA model seems to show a larger separation in accordance with the experiments. However, at $Re_{2s} = 2.1 \cdot 10^5$ the SST- γ - Re_θ model captures better the small separation bubble.

Finally, the models are evaluated in terms of mass averaged exit kinetic losses and angle, as reported in Figure 16. As observed for the T106c, even in this case the ANN augmented SA model outperforms the original SA model at low Reynolds numbers. It is interesting to note that the numerical results obtained in the present work presents an offset in β_2 with respect to the experimental results, offset which is not observed in the results obtained from the SST- γ - Re_θ model. This could be a limitation of the SA model which is inherited by the augmented model: future work will be devoted to apply the field inversion approach to other RANS models to verify whether this limitation persists.

8. Conclusions

The potential of the field inversion approach was investigated for the augmentation of a RANS model used in the simulation of turbomachinery flows. In particular the approach was applied to the original SA model and the

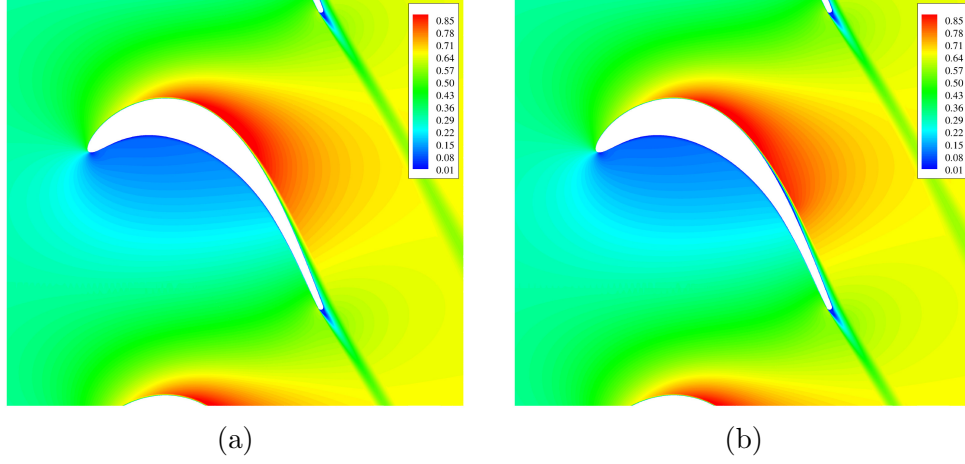


Figure 14: Mach field for the T2 cascade at $Re_{2s} = 2.1 \cdot 10^5$ with the original SA model (a) and with the ANN-SA model (b)

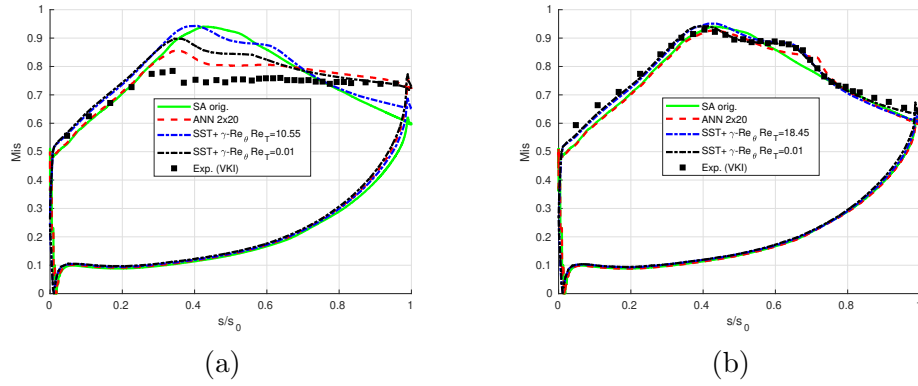


Figure 15: Mis distribution for T2 cascade at $Re_{2s} = 1.2 \cdot 10^5$ (a) and $Re_{2s} = 2.1 \cdot 10^5$ (b): comparison between original SA model, SA-ANN model and experimental results

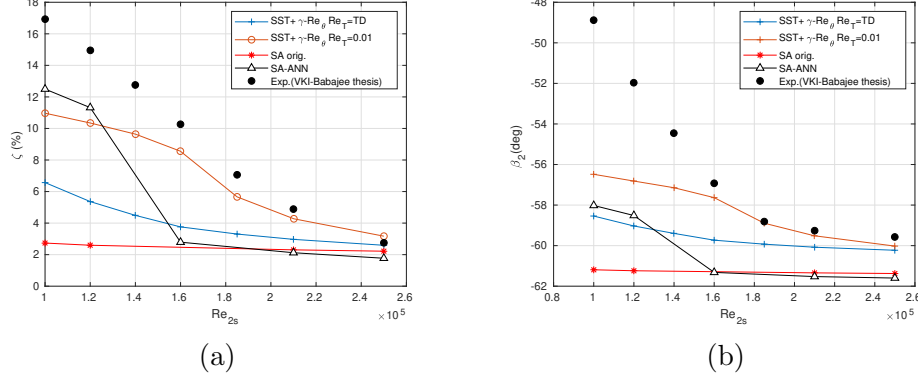


Figure 16: Average losses and exit angle for T2 cascade: comparison between original SA model, SA-ANN model and experimental results

attention is focused on transitional flows with separation in low pressure gas turbines. Since the original model is not suited for this kind of flows, the field inversion approach is used to develop a local correction of the production term which acts like an intermittency correction for transitional flows. The correction factor is then expressed by means of an ANN as a function of some physical quantities in order to generalise the model. An investigation has been carried out on the definition of the input features which are improved with respect to the original definitions suggested in the literature. A convergence study is carried out to choose the architecture of the ANN in order to underline the problem of overfitting. The ability of the ANN augmented SA model to compute low Reynolds number flow fields in low pressure gas turbine cascades is investigated by performing actual predictions at different Reynolds numbers and on a different geometry with respect to the one used for the field inversion. Furthermore, a new expression of the correction term is proposed in order to limit its value in a finite range: this, together with the introduction of a limiting on input features, significantly improves the robustness of the approach during transients and in predictions.

The results seem promising and are substantially better than the results provided by the original model. They also appears satisfactory if compared to the results obtained by a significantly more complex four equation model (SST- γ - Re_θ). In particular, even if the goal function used for the field inversion is based only on the wall isentropic Mach number, the ANN augmented model shows improvements also in terms of average losses and exit angle in the wake.

718 Future work will be devoted to the application of the field inversion ap-
719 proach to other RANS models. Furthermore, possible alternatives to the use
720 of an ANN will be investigated for achieving a better fitting of the database
721 with a good level of robustness in predictions.

722 9. Acknowledgements

723 Computational resources were provided by HPC@POLITO, a project of
724 Academic Computing within the Department of Control and Computer En-
725 gineering at the Politecnico di Torino (<http://www.hpc.polito.it>).
726 We acknowledge the CINECA award under the ISCRA initiative, for the avail-
727 ability of high performance computing resources and support. The simula-
728 tions were performed on the Marconi Tier-0 System for the Project FIRST.

729 References

- 730 [1] S. Russo, P. Luchini, A fast algorithm for the estimation of statistical
731 error in DNS (or experimental) time averages, *Journal of Computational*
732 *Physics* 347 (2017) 328–340.
- 733 [2] R. D. Sandberg, V. Michelassi, The current state of high-fidelity simula-
734 tions for main gas path turbomachinery components and their industrial
735 impact, *Flow, Turbulence and Combustion* 102 (4) (2019) 797–848.
- 736 [3] X. Xie, M. Mohebbujjaman, L. G. Rebholz, T. Iliescu, Data-driven fil-
737 tered reduced order modeling of fluid flows, *SIAM Journal on Scientific*
738 *Computing* 40 (3) (2018) B834–B857.
- 739 [4] R. Dupuis, J.-C. Jouhaud, P. Sagaut, Surrogate modeling of aerody-
740 namic simulations for multiple operating conditions using machine learn-
741 ing, *AIAA Journal* 56 (9) (2018) 3622–3635.
- 742 [5] L. Margheri, M. Melli, M. V. Salvetti, P. Sagaut, Epistemic uncertain-
743 ties in RANS model free coefficients, *Computers & Fluids* 102 (2014)
744 315–335.
- 745 [6] A. Ferrero, A. Iollo, F. Larocca, Reduced order modelling for turbo-
746 machinery shape design, *International Journal of Computational Fluid*
747 *Dynamics* (2019) 1–12.

- 748 [7] A. Ferrero, A. Iollo, F. Larocca, Global and local POD models for the
749 prediction of compressible flows with DG methods, *International Journal*
750 *for Numerical Methods in Engineering* 116 (5) (2018) 332–357.
- 751 [8] M. Bergmann, A. Ferrero, A. Iollo, E. Lombardi, A. Scardigli, H. Telib,
752 A zonal galerkin-free POD model for incompressible flows, *Journal of*
753 *Computational Physics* 352 (2018) 301–325.
- 754 [9] M. Raissi, G. E. Karniadakis, Hidden physics models: Machine learn-
755 ing of nonlinear partial differential equations, *Journal of Computational*
756 *Physics* 357 (2018) 125–141.
- 757 [10] J.-X. Wang, J.-L. Wu, H. Xiao, Physics-informed machine learning ap-
758 proach for reconstructing Reynolds stress modeling discrepancies based
759 on DNS data, *Physical Review Fluids* 2 (3) (2017) 034603.
- 760 [11] J. Weatheritt, R. Sandberg, A novel evolutionary algorithm applied to
761 algebraic modifications of the RANS stress–strain relationship, *Journal*
762 *of Computational Physics* 325 (2016) 22–37.
- 763 [12] J. Weatheritt, R. Pichler, R. D. Sandberg, G. Laskowski, V. Michelassi,
764 Machine learning for turbulence model development using a high-fidelity
765 HPT cascade simulation, in: *ASME Turbo Expo 2017: Turbomachinery*
766 *Technical Conference and Exposition*, American Society of Mechanical
767 Engineers Digital Collection, 2017, p. 12.
- 768 [13] K. Duraisamy, Z. J. Zhang, A. P. Singh, New approaches in turbulence
769 and transition modeling using data-driven techniques, in: *53rd AIAA*
770 *Aerospace Sciences Meeting*, 2015, p. 1284.
- 771 [14] E. J. Parish, K. Duraisamy, A paradigm for data-driven predictive mod-
772 eling using field inversion and machine learning, *Journal of Computa-*
773 *tional Physics* 305 (2016) 758–774.
- 774 [15] F. Gibou, D. Hyde, R. Fedkiw, Sharp interface approaches and deep
775 learning techniques for multiphase flows, *Journal of Computational*
776 *Physics* 380 (2019) 442–463.
- 777 [16] H. Patel, A. Panda, J. Kuipers, E. Peters, Computing interface curva-
778 ture from volume fractions: A machine learning approach, *Computers*
779 *& Fluids* 193 (2019) 104263.

- 780 [17] A. Takbiri-Borujeni, M. Ayoobi, Application of physics-based machine
781 learning in combustion modeling, in: 11th US National Combustion
782 Meeting, 2019, p. 10.
- 783 [18] S. Bhalla, M. Yao, J.-P. Hickey, M. Crowley, Compact representation of
784 a multi-dimensional combustion manifold using deep neural networks,
785 in: European Conference on Machine Learning, 2019, p. 16.
- 786 [19] X. Zhu, Z. Cai, J. Wu, Y. Cheng, Q. Huang, Convolutional neural net-
787 work based combustion mode classification for condition monitoring in
788 the supersonic combustor, *Acta Astronautica* 159 (2019) 349–357.
- 789 [20] Y.-P. Zhao, Q.-K. Hu, J.-G. Xu, B. Li, G. Huang, Y.-T. Pan, A robust
790 extreme learning machine for modeling a small-scale turbojet engine,
791 *Applied energy* 218 (2018) 22–35.
- 792 [21] Z. Liu, I. A. Karimi, Gas turbine performance prediction via machine
793 learning, *Energy* (2019) 116627.
- 794 [22] K. Duraisamy, G. Iaccarino, H. Xiao, Turbulence modeling in the age of
795 data, *Annual Review of Fluid Mechanics* 51 (2019) 357–377.
- 796 [23] S. R. Allmaras, F. T. Johnson, Modifications and clarifications for the
797 implementation of the Spalart-Allmaras turbulence model, in: Seventh
798 international conference on computational fluid dynamics (ICCFD7),
799 2012, pp. 1–11.
- 800 [24] A. Ferrero, A. Iollo, F. Larocca, RANS closure approximation by artifi-
801 cial neural networks, in: 13 th European Conference on Turbomachinery
802 Fluid dynamics & Thermodynamics, EUROPEAN TURBOMACHIN-
803 ERY SOCIETY, 2019, p. 14.
- 804 [25] R. Hartmann, P. Houston, Adaptive discontinuous galerkin finite ele-
805 ment methods for the compressible Euler equations, *Journal of Compu-*
806 *tational Physics* 183 (2) (2002) 508–532.
- 807 [26] J.-F. Remacle, J. E. Flaherty, M. S. Shephard, An adaptive discontinu-
808 ous galerkin technique with an orthogonal basis applied to compressible
809 flow problems, *SIAM review* 45 (1) (2003) 53–72.

- [27] G. Zenoni, T. Leicht, A. Colombo, L. Botti, An agglomeration-based adaptive discontinuous Galerkin method for compressible flows, *International Journal for Numerical Methods in Fluids* 85 (8) (2017) 465–483.
- [28] A. Ferrero, F. Larocca, V. Bernaschek, Unstructured discretisation of a non-local transition model for turbomachinery flows, *Advances in aircraft and spacecraft science* 4 (5) (2017) 555–571.
- [29] A. Burbeau, P. Sagaut, A dynamic p-adaptive discontinuous galerkin method for viscous flow with shocks, *Computers & fluids* 34 (4-5) (2005) 401–417.
- [30] G. Giorgiani, S. Fernández-Méndez, A. Huerta, Hybridizable discontinuous galerkin p-adaptivity for wave propagation problems, *International Journal for Numerical Methods in Fluids* 72 (12) (2013) 1244–1262.
- [31] E. Ampellio, F. Bertini, A. Ferrero, F. Larocca, L. Vassio, Turbomachinery design by a swarm-based optimization method coupled with a CFD solver, *Advances in aircraft and spacecraft science* 3 (2) (2016) 149.
- [32] C. Eskilsson, An hp-adaptive discontinuous Galerkin method for shallow water flows, *International Journal for Numerical Methods in Fluids* 67 (11) (2011) 1605–1623.
- [33] A. Ferrero, F. Larocca, Adaptive CFD schemes for aerospace propulsion, in: *Journal of Physics: Conference Series*, Vol. 841, IOP Publishing, 2017, p. 012017.
- [34] N. Chalmers, G. Agbaglah, M. Chrust, C. Mavriplis, A parallel hp-adaptive high order discontinuous Galerkin method for the incompressible Navier-Stokes equations, *Journal of Computational Physics: X* 2 (2019) 100023.
- [35] C. Geuzaine, J.-F. Remacle, Gmsh: A 3-d finite element mesh generator with built-in pre-and post-processing facilities, *International journal for numerical methods in engineering* 79 (11) (2009) 1309–1331.
- [36] M. Lange, M. G. Knepley, G. J. Gorman, Flexible, scalable mesh and data management using PETSc DMplex, in: *Proceedings of the 3rd International Conference on Exascale Applications and Software*, University of Edinburgh, 2015, pp. 71–76.

- [37] S. Balay, S. Abhyankar, M. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. Gropp, et al., PETSc users manual (2019).
- [38] F. Bassi, L. Botti, A. Colombo, D. A. Di Pietro, P. Tesini, On the flexibility of agglomeration based physical space discontinuous galerkin discretizations, *Journal of Computational Physics* 231 (1) (2012) 45–65.
- [39] S. Osher, F. Solomon, Upwind difference schemes for hyperbolic systems of conservation laws, *Mathematics of computation* 38 (158) (1982) 339–374.
- [40] M. Pandolfi, A contribution to the numerical prediction of unsteady flows, *AIAA journal* 22 (5) (1984) 602–610.
- [41] A. Ferrero, F. Larocca, G. Puppo, A robust and adaptive recovery-based discontinuous Galerkin method for the numerical solution of convection–diffusion equations, *International Journal for Numerical Methods in Fluids* 77 (2) (2015) 63–91.
- [42] F. Bassi, L. Botti, A. Colombo, A. Crivellini, N. Franchina, A. Ghidoni, S. Rebay, Very high-order accurate discontinuous galerkin computation of transonic turbulent flows on aeronautical configurations, in: *ADIGMA-A European Initiative on the Development of Adaptive Higher-Order Variational Methods for Aerospace Applications*, Springer, 2010, pp. 25–38.
- [43] A. Ferrero, F. Larocca, Feedback filtering in discontinuous Galerkin methods for Euler equations, *Progress in Computational Fluid Dynamics, an International Journal* 16 (1) (2016) 14–25.
- [44] A. P. Singh, S. Medida, K. Duraisamy, Machine-learning-augmented predictive modeling of turbulent separated flows over airfoils, *AIAA Journal* (2017) 2215–2227.
- [45] C. M. Bishop, Training with noise is equivalent to tikhonov regularization, *Neural computation* 7 (1) (1995) 108–116.
- [46] L. Hascoet, V. Pascual, The Tapenade automatic differentiation tool: Principles, model, and specification, *ACM Transactions on Mathematical Software (TOMS)* 39 (3) (2013) 20.

- [47] K. Duraisamy, P. Durbin, Transition modeling using data driven approaches, in: CTR Summer Program, 2014, p. 427.
- [48] J. Michalek, M. Monaldi, T. Arts, Aerodynamic performance of a very high lift low pressure turbine airfoil (T106C) at low Reynolds and high Mach number with effect of free stream turbulence intensity, *Journal of Turbomachinery* 134 (6) (2012) 061009.
- [49] 2nd international workshop on high-order CFD methods, https://www.dlr.de/as/desktopdefault.aspx/tabid-8170/13999_read-35550/, accessed: 2019-12-02 (2013).
- [50] J. Babajee, Detailed numerical characterization of the separation-induced transition, including bursting, in a low-pressure turbine environment, Ph.D. thesis, Ecole Centrale de Lyon; Institut von Karman de dynamique des fluides (2014).
- [51] J. Hourmouziadis, Aerodynamic design of low pressure turbines, AGARD, Blading Design for Axial Turbomachines 40 p(SEE N 89-27661 22-07) (1989).
- [52] P. R. Spalart, S. Deck, M. L. Shur, K. D. Squires, M. K. Strelets, A. Travin, A new version of detached-eddy simulation, resistant to ambiguous grid densities, *Theoretical and computational fluid dynamics* 20 (3) (2006) 181.
- [53] F. D. Foresee, M. T. Hagan, Gauss-newton approximation to bayesian learning, in: *Proceedings of International Conference on Neural Networks (ICNN'97)*, Vol. 3, IEEE, 1997, pp. 1930–1935.
- [54] A. Benyahia, L. Castillon, R. Houdeville, Prediction of separation-induced transition on high lift low pressure turbine blade, in: *ASME 2011 Turbo Expo: Turbine Technical Conference and Exposition*, American Society of Mechanical Engineers Digital Collection, 2011, pp. 1835–1846.
- [55] C. Content, R. Houdeville, Application of the γ - $r\theta$ laminar-turbulent transition model in Navier-Stokes computations, in: *40th Fluid Dynamics Conference and Exhibit*, 2010, p. 4445.

- 905 [56] R. Pacciani, M. Marconcini, A. Arnone, F. Bertini, A CFD study of
906 low Reynolds number flow in high lift cascades, in: ASME Turbo Expo
907 2010: Power for Land, Sea, and Air, American Society of Mechanical
908 Engineers Digital Collection, 2010, pp. 1525–1534.
- 909 [57] F. R. Menter, R. B. Langtry, S. Likki, Y. Suzen, P. Huang, S. Völker, A
910 correlation-based transition model using local variables—part I: model
911 formulation, *Journal of turbomachinery* 128 (3) (2006) 413–422.
- 912 [58] R. B. Langtry, F. Menter, S. Likki, Y. Suzen, P. Huang, S. Völker, A
913 correlation-based transition model using local variables—part II: test
914 cases and industrial applications, *Journal of Turbomachinery* 128 (3)
915 (2006) 423–434.