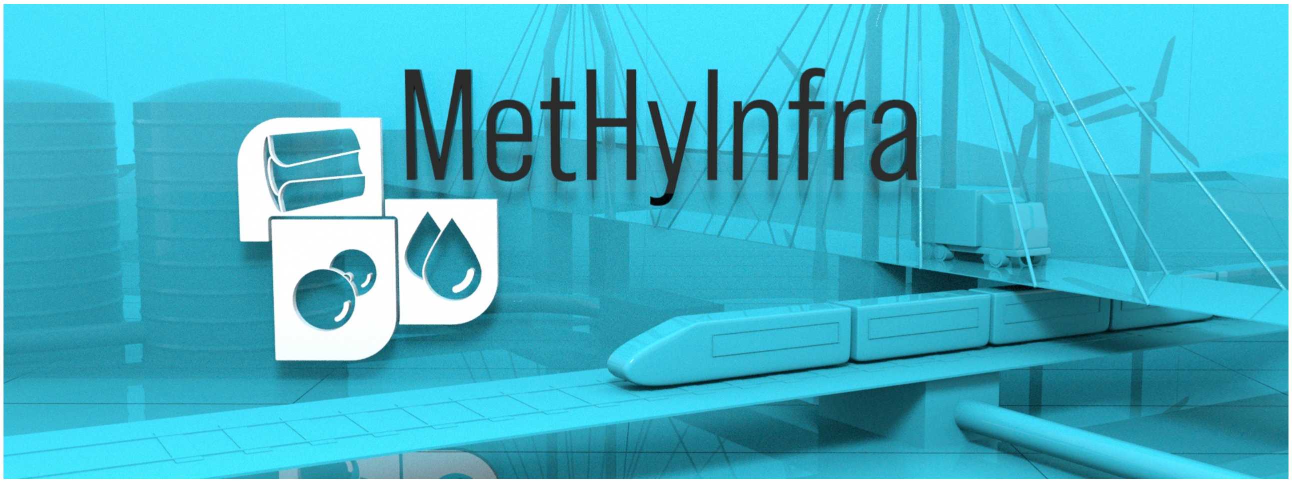

REPORT:
Suitable turbulence models for high-pressure hydrogen flows through critical nozzles

A3.1.3: Report of literature review

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Summary

This report on suitable turbulence modeling approaches for the simulation of high-pressure hydrogen flows through critical nozzles was written as part of activity 3.1.3 from the EMPIR Metrology infrastructure for high-pressure gas and liquified hydrogen flows (MetHyInfra) project. The three-year European project commenced on 1st June 2021 and focused on providing metrological infrastructure and traceability for high pressure hydrogen flow meter calibration (1000 bar / 3.6 kg/min), fuel cells applications (4 kg/h, 30 bar) and liquid hydrogen. For more details about this project please visit methyinfra.ptb.de.

This report reviews several turbulence modeling approaches in the context of simulating high-pressure hydrogen flows through critical nozzles. It summarizes the relevant flow effects that need to be captured by the turbulence model, presents several modeling approaches from the literature, and reviews them.

Confidentiality	Public

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Contents

1 Introduction

This report summarizes the Activity A3.1.3 of the EMPIR 20IND11 MetHyInfra project. A literature study was performed on suitable turbulence models for the numerical simulation of high-pressure hydrogen flows (up to 100 MPa) for Reynolds number ranges up to $5 \cdot 10^6$ through critical flow Venturi nozzles. Different turbulence modeling approaches are reviewed and compared in this report.

The main goal of this literature study is to find an appropriate turbulence modeling approach for the flow through critical nozzles. Therefore, the focus of this review was rather on the direct application of turbulence models for this specific flow scenario in recent investigations than on the general description of turbulence models available.

In general, high-pressure flows through critical nozzles can be described by the following flow effects, the turbulence model needs to be able to capture:

- compressibility effects, e. g. shock structures
- boundary layer effects, e. g. development of displacement thickness
- transitional effects, e. g. prediction of laminar-to-turbulent transition
- wall effects, e. g. due to the influence of rough walls and heat transfer

Furthermore, the turbulence modeling strategy should be selected according to an appropriate compromise between computational runtime and accurate prediction of relevant flow physics.

Turbulence modeling approaches can be classified into the following three main groups:

- RANS (Reynolds-averaged Navier-Stokes)
- LES (Large Eddy Simulation)
- Hybrid (combination of RANS and LES)

In the following, those turbulence models are presented in the context of various numerical investigations addressing flow cases that are comparable to those in the MetHyInfra project.

2 RANS turbulence models

RANS turbulence models can be divided into the following three main groups: linear eddy viscosity models, non-linear eddy viscosity models, and Reynolds stress transport models. They all have in common that they use modeling approaches to solve the closure problem in terms of the Reynolds stress tensor. Linear eddy viscosity models assume a linear dependency between the Reynolds stress tensor and the mean velocity field (Boussinesq hypothesis). There are several subcategories of linear eddy-viscosity models, depending on the number of (transport) equations that need to be solved to compute the eddy viscosity. Examples for linear eddy-viscosity models are the Spalart-Allmaras model (one-equation model), the k-ϵ, k-ω, or k-ω shear stress transport (SST) model (two-equation models). Non-linear eddy viscosity extend the equation that models the turbulent Reynolds stresses by non-linear terms. This group of models also includes explicit algebraic Reynolds stress models. Reynolds stress transport models (often only called Reynolds stress models and hence abbreviated by RSM) directly compute the six different components of the Reynolds stress tensor via the exact Reynolds stress transport equations, where modeling is required for the contributing terms involved. Thus, they are able to account for complex interactions in turbulent flow fields, such as the directional effects of the Reynolds stresses.

In the following section, the use of classical RANS models in recent numerical investigations of critical nozzle flow will be presented. In Subsection 2.2, transitional RANS models, which incorporate additional transport equations in order to predict laminar-to-turbulent transition, will be introduced. Furthermore, the performance of these models compared to classical RANS models will be shown for several nozzle flow applications.

2.1 Classical RANS turbulence models

Balabel et al. [1] numerically investigated the gas flow through a two-dimensional convergent-divergent rocket nozzle for different nozzle pressure ratios using six different RANS turbulence models. Their comparison comprises the standard k-ϵ model, the extended k-ϵ model, the shear-stress transport k-ω model, an RSM, the v2-f and the realizable v2-f model. The SST k-ω and the realizable v2-f models provided the best results regarding the prediction of the shock wave position as well as the separation point. According to the authors, the gradual change of the SST model from the standard k-ω model in the inner region of the boundary layer to the k-ϵ model in the outer part of it might be the reason for the good performance. With respect to computational time, the high-Re SST turbulence model was recommended for nozzle flow problems. Furthermore, for this model, comparisons with experimental data regarding the shock schematic (e. g., shock angle, Mach disc width, etc.) were in good accordance.

Giglmaier et al. [4] compared four different eddy viscosity models and six different Reynolds stress models for the flow simulation of a pseudo-shock system in a planar nozzle. All models were used with the standard settings in ANSYS CFX. Based on their results of the Mach number distribution in the symmetry plane and pressure distribution at the walls in comparison with experimental data, they divided their findings into three groups. First, the Spalart-Allmaras and the SST turbulence model showed an nonphysical long pseudo-shock system and the positions of shock and pressure distribution did not fit the experiment. Second, the k-ω model and the three ω-based RSM showed a similar pseudo-shock system and the shock position was slightly shifted downstream compared to the experiment. Third, the k-ϵ model and the ϵ-based RSM predicted the primary shock further upstream and no recirculation zone was established at the channel wall. Although the SST model is an approach that combines the advantages of the k-ϵ and k-ω models, their results of the SST model were worse than those observed with both other models. The SST model includes a limiter for the eddy viscosity that was introduced in order to improve the prediction of boundary layer separation. In their specific case the limiter led to an under-prediction of the eddy viscosity and therefore the model failed to predict flow separation. Nevertheless, they did not further investigate this topic in their paper.

Ünsal and Çalışkan [25] studied the discharge coefficient dependency on Reynolds number and wall temperature for toroidal critial flow Venturi nozzles (CFVNs) using a two-dimensional axisymmetric simulation model in the CFD software package ANSYS Fluent. For their simulations, they used the k-ϵ with enhanced wall treatment and the SST turbulence model since those models are able to obtain laminar boundary layers and also capture supersonic separation along the divergent part of the nozzle. Furthermore, they mentioned the benefit of RANS models in terms of reasonable computation time in comparison with LES or DNS (direct numerical simulation) approaches. Over a broad range of Reynolds numbers, their resulting discharge coefficient showed good agreement with ISO 9300 and correlation curves based on experimental data by Ishibashi [5]. According to the authors, the numerical modeling was able to predict the boundary layer and thus helps to improve the understanding of the sonic nozzle flow field.

Tharwat et al. [19] simulated the flow through a dual throat nozzle at a pressure ratio of 4. They used the SST k-ω and the standard k-ϵ model and compared their results with experiments of the NASA Langley research center. The standard k-ϵ model showed good agreement with the measurement results in the pressure recovery zone of the nozzle. However, it predicted weak flow separation. The SST model over-predicted the separation behavior in the divergent part of the nozzle and thus under-predicted the pressure recovery. For the SST model, the stress structure parameter a_1 was investigated regarding the prediction of the pressure distribution. This parameter is used as a limiter of the turbulent shear stress in relation to the turbulent kinetic energy. They showed an improved prediction of the pressure recovery for a value of $a_1 = 0.34$ (in comparison to the default value of 0.31).

Knopp [8] developed modifications of RANS turbulence models for a better prediction of low-speed flow separation on airfoils and wings near stall. Their modifications were based on a proposal for a new wall-law for the mean velocity in the inner layer of a turbulent boundary layer at adverse pressure gradient. The wall-law is described with a log-law in the inner part and with a half-power (or square-root) law in the outer part of the inner layer of the turbulent boundary layer. For the SST model, they modified the equations of k and ω such that the wall-law (as described above) is satisfied. Those modifications regarding the wall-laws were calibrated with a large experimental database, thus making the modified turbulence model more sensitive to flow separation by a reduction of the turbulent shear stress in the near wall region.
Likewise, Knopp et al. [9] modified the ω-equation of the SSG/LLR-ω model, which belongs to the group of RSMs, and compared it to a new experiment of a turbulent boundary layer flow with a large adverse pressure gradient at a high Reynolds number. For the modified model, an improved agreement with experimental data was found.

Masgo [14] evaluated five different turbulence models for the flow of air in a planar nozzle including the SST k-ω, standard k-ϵ, standard k-ω, transition k-kl-ω and RSM model. Two pressure ratios (total inlet to static outlet), namely 2.008 and 3.413, were analyzed. Comparing the static pressure profiles at the nozzle walls and the forms of the shock wave in the flow field, the SST k-ω model obtained the best fit to corresponding experimental data. This is in accordance with the work by Balabel et al. [1] described above.

Kim et al. [7] studied the influence of different real gas and turbulence models on the discharging process of a high-pressure gaseous hydrogen tank using the CFD package ANSYS Fluent. The different turbulence models analyzed were the realizable k-ϵ, RNG k-ϵ, SST, and RSM models. The SST model results showed the closest agreement with corresponding experimental data regarding the gas temperature during discharging, whereas the realizable k-ϵ model gave poor predictions. In terms of the turbulence intensity, the SST and RSM predicted lower values than the realizable k-ϵ and RNG models.

2.2 Transitional RANS turbulence models

Langtry and Menter [10] and Menter et al. [15] developed a correlation-based transition model that is strictly based on local variables. Thus, it is applicable to any CFD code. This specifically includes unstructured grids and parallelization. The model extends the k-ω SST turbulence model by two additional transport equations, one for the intermittency γ and one for the momentum thickness Reynolds number Re_θ. The latter one is a criterion for the onset of transition from laminar to turbulent flow. The intermittency is used to trigger the transition process, where a value of $\gamma = 0$ and $\gamma = 1$ corresponds to laminar and turbulent flow, respectively. The second transport equation for Re_θ includes experimental correlations that are typically based on freestream values, like the turbulence intensity or the pressure gradient outside the boundary layer. The model is therefore often referenced as the γ-Re_θ transition model.

Kaynak et al. [6] elaborated the transitional Bas-Cakmakcioglu (B-C) algebraic model for a number of two- and three-dimensional test cases (flat plate, airfoil, turbomachinery blades, etc.) with promising results. The B-C model incorporates an algebraic γ-function (in contrast to the intermittency transport equation in the model by Langtry and Menter [10] and Menter et al. [15]) into the one-equation Spalart-Allmaras turbulence model. Thus, it portrays a leaner formulation of a transitional model without the need of additional transport equations.

Malan et al. [12] described the implementation of the γ-Re_θ transition model by Langtry and Menter [10] and Menter et al. [15] in a commercial CFD code (STAR-CCM+) and the process of calibrating the main correlations with experimental data. At this time, in 2009, two key correlations, $Re_{\theta c}$ and F_{length}, were kept proprietary, so that they synthesized those correlations in order to help others perform similar calibrations. They applied their synthesized correlations to several validation cases, i. e. flat plate, airfoil and turbomachinery flows and showed favorable agreement with those of Langtry [11]. Further, they highlighted that the computational cost is significantly higher than fully turbulent calculations due to more demanding mesh requirements and the higher convergence time with two additional transport equations. Nonetheless, their successful application to a realistic industrial flow simulation valued the approach.

Ünsal et al. [24] computationally examined the boundary layer transition of toroidal critical flow Venturi nozzles in ANSYS Fluent. They used the k-ϵ model with enhanced wall treatments as well as the SST model using its ability to model intermittency to predict transition with automatic wall functions. Based on their results, boundary layer transition took place within the diffuser section of the nozzle for low Reynolds numbers. With increasing Reynolds number, the transition position moved upstream up to the nozzle inlet section. In terms of the discharge coefficient variation, their results (red dots) were in good accordance with an empirical curve (sCurve) proposed by Ishibashi [5] in the laminar and turbulent region (see Fig. 1). However, their estimated transitional location ($Re_{tr} \approx 3.5 \cdot 10^6$) is higher than the empirical curve (sCurve) predicts ($Re_{tr} \approx 1 \cdot 10^6$).

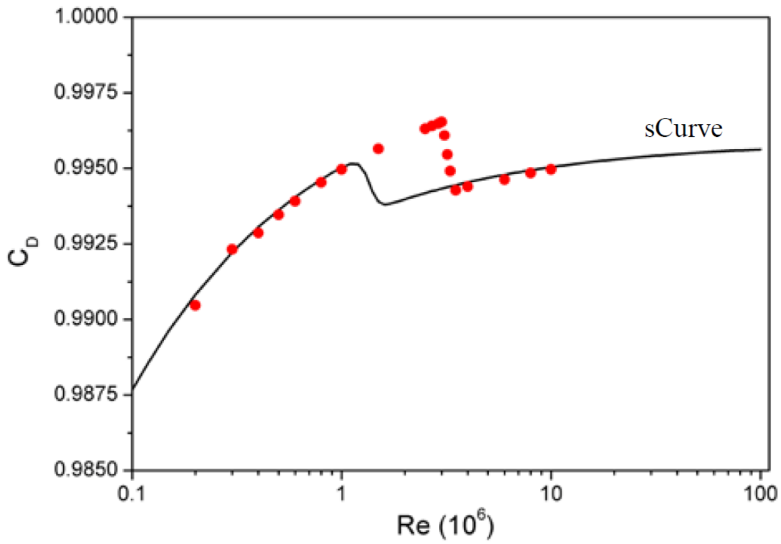

Figure 1: Variation of the discharge coefficient with Reynolds number. Red dots: simulation results by Ünsal et al. [24], black line: theoretical prediction (sCurve) by Ishibashi [5]. Picture taken from [24].

Nakhostin [17] investigated transitional turbulence models for the prediction of the drag crisis in flows over spheres and cylinders. The turbulence models used were the k-ω SST and the γ-Re_θ transition model. Furthermore, a DES (Detached Eddy Simulation) version of the γ-Re_θ transition model was implemented in OpenFOAM, called kOmegaSSTLMDES. In terms of the drag coefficient, the DES and RANS results are very similar, so that the time-dependent behavior of the vortices did not significantly influence the mean drag. However, the DES provided additional information regarding the vortex shedding. For the sphere and cylinder cases, the difference between the fully turbulent and the transitional model was small for lower Reynolds numbers, whereas at the highest Reynolds number simulated, the transitional model showed closer accordance to experimental data than the fully turbulent model.

Wang et al. [21] investigated the influence of wall roughness on boundary layer transition position in toroidal critical flow Venturi nozzles. They conducted a series of numerical simulations using the γ-Re_θ transition model for different nozzle diameters and sand roughness values. Their results were in line with the ISO 9300 empirical equation and corresponding experimental data. The boundary layer transition location was directly affected by the wall roughness that was represented by an earlier drop in discharge coefficient for higher roughness values.

3 Hybrid and LES turbulence models

In contrast to RANS models, LES does not use time- or ensemble-averaging to obtain the Reynolds stresses. In LES, the large scale motions of the turbulent flow (large eddies) are computed directly, whereas the small scale structures (sub-grid scale – SGS) are modeled. This results in a significant reduction of computational costs compared to DNS. On the other hand, LES is more accurate than RANS since the large eddies, which contain most of the turbulent energy and, hence, are responsible for most of the momentum transfer and turbulent mixing, are captured in full detail. However, LES is also much more computationally expensive than RANS because a much finer grid is needed to resolve the large eddies. Hybrid models, like detached eddy simulation (DES) or delayed detached eddy simulation (DDES) are a "compromise" between RANS and LES models. The idea of these models is to combine the RANS technology in the boundary layers (where an large eddy simulation (LES) would be too costly) with an LES in the separated regions.

Ghosh et al. [3] analyzed effects of extra strain and dilatation rates on the turbulence structure in axisymmetric nozzles and diffusers with fully developed supersonic pipe flow as inflow condition by means of LES with high-order numerical schemes. Their LES results were also validated with DNS results of pipe and nozzle flows for selected flow cases. They found that weak pressure gradients already strongly inhibit or enhance the Reynolds stresses via corresponding changes of production and pressure-strain terms. Those results depict a database for the improvement of second-order turbulence models for compressible flow.

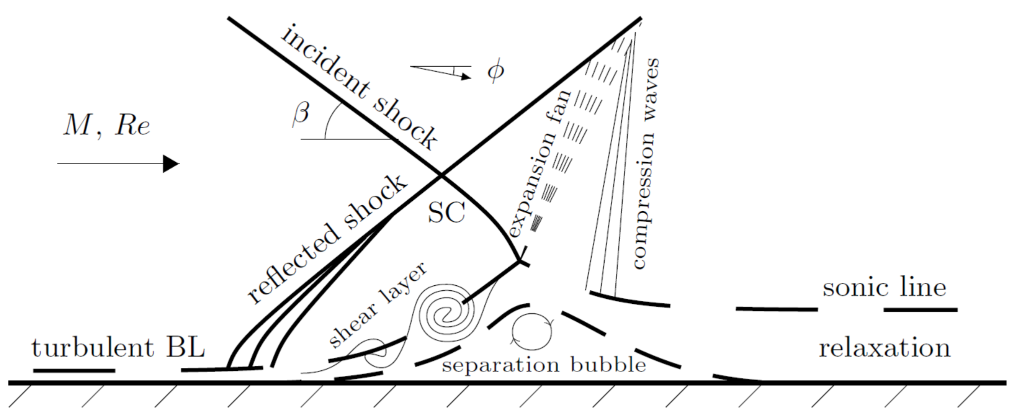

Figure 2: Schematic diagram of the shock-turbulent-boundary-layer interaction. M and Re are the Mach and Reynolds numbers of the incoming flow, respectively; β is the incident shock angle; ϕ is the deflection angle experienced by the flow when traversing the incident shock; SC is the shock-crossing point, defined as the intersection between the incident and reflected shocks. The presence of a separation bubble is dependent on the strengths of the adverse pressure gradient resulting from the interaction and the incoming turbulent boundary layer. Picture taken from [2].

Bermejo-Moreno et al. [2] investigated the interaction of an oblique shock and a turbulent boundary layer (as schematically illustrated in Fig. 2) in a low aspect-ratio duct using wall-modeled LES and compared their results with particle image velocimetry (PIV) measurements. In addition, they also studied the three-dimensional effects caused by the presence of the side walls. Results between simulation and experiment were compared in terms of mean and turbulent quantities at four different planes parallel to the side walls. The flow features of the interaction and three-dimensional effect were well captured by the simulation and the prediction of the shock-angle of the incident shock was within 5 % of the corresponding experimental value. This discrepancy was presumably due to the thinner boundary layer resulting from the LES. However, the profiles of mean stream-wise and wall-normal velocities were in good accordance with the experimental data.

Mousavi and Roohi [16] investigated the behavior of the shock train in a convergent-divergent nozzle numerically using different turbulence models. They compared two eddy-viscosity RANS models (k-ε RNG and k-ω SST) with a RSM as well as with LES. Comparison of the simulation results with experimental data by Weiss et al. [23] showed that, the LES simulation is more accurate compared to the other models. However, the authors also report that, the computational costs for the LES are around 11 times higher compared to the RSM and approximately 17 times higher compared to the eddy-viscosity RANS models.

Quaatz et al. [18] conducted a well-resolved LES of a pseudo-shock system in the divergent part of a Laval nozzle with rectangular cross-section and compared their results with a reference experimental setup. Their simulation results were in excellent agreement with wall pressure measurements and experimental Schlieren visualizations. Further, they analyzed the performance of several standard two-equation RANS models in predicting pseudo-shock systems in turbulent duct flows using their LES data as a reference. They supported the conclusions of Giglmaier et al. [4] about the superior performance of explicit algebraic Reynolds stress models in comparison with linear eddy viscosity models.

Martelli et al. [13] simulated a three-dimensional planar overexpanded nozzle by means of the Delayed Detached Eddy Simulation (DDES) technique and compared their results with corresponding experiments and LES studies from literature. The nozzle flow was characterized by a strong non-symmetric separation shock with a classical lambda shape and by an important recirculation zone. The pressure signals were analyzed by wavelet decomposition and their peak values were in accordance with those of the LES and experiment. In contrast, the excursion length of the shock was too high compared with the LES and experimental values.

Wang and McGuirk [22] developed an LES methodology for the simulation of accelerated nozzle flows with the aim to predict the re-laminarisation of the flow in the convergent and parallel part of the nozzle. They compared two different subgrid scale (SGS) models: the Smagorinsky model and the Piomelli and Geurts model. For the latter one, they adapted one of the model coefficients in such a way that, the error in the prediction of the integral length scale in a zero pressure gradient boundary layer is minimized. Wang and McGuirk [22] validated their simulation results by comparison with experimental data from Trumper et al. [20]. Both LES approaches predict boundary layer parameters (like boundary layer thickness δ, momentum thickness θ, shape factor H_{12}, or Reynolds number Re_θ) at the nozzle in- and outlet very well compared to the experiment. However, comparison with measured exit turbulence characteristics revealed a considerable improvement with the Piomelli and Guerts model. Both amplitude and location of the peak stress and the overall profile shape were better predicted. Considering mean velocity profiles at the nozzle exit, both LES approaches show close agreement with experimental data. Furthermore, the LES results show an improvement compared to low Re RANS predictions (by means of the Launder-Sharma model).

4 Conclusion

In this report, several turbulence modeling approaches for the simulation of the flow through critical nozzles have been reviewed. For this application, RANS models (and especially linear eddy viscosity models) are the most commonly used turbulence models. LES has previously been applied more rarely and mainly if the focus of the investigation was on the modeling of the shock structures and boundary layer effects. A comparison between (classical) RANS and LES for these cases shows that the LES results are usually closer to experimental data than the RANS predictions. However, the computational costs for an LES are also much higher than for a RANS simulation. Furthermore, to the authors' knowledge, no comparison between transitional RANS models and LES has been performed so far.

Transitional RANS models incorporate additional transport equations for predicting the transition from laminar to turbulent flow. Hence, these models are more suitable for modeling transitional effects than classical RANS models. For an appropriate modeling of the effect of rough walls, a turbulence model needs to be chosen that allows the inclusion of wall roughness parameters, e. g., in its wall functions.

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