TURBULENCE MODELS BASED ON THE LENGTH-SCALE EQUATION

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ABSTRACT

The different formulations of Scale-Adaptive Simulation (SAS) turbulence models will be presented. The physical motivation behind the SAS concept will be given and illustrated for generic and technical flows. Some practical advantages of SAS versus DES will be discussed.

INTRODUCTION

There is a growing understanding in industrial CFD that unsteady simulations are required for a wide range of technical flows. There are two categories of flows where steady-state simulations are not sufficient for providing the information required by design engineers:

* Category I: Flows, where steady-state simulations are not of sufficient accuracy and do not properly describe the true nature of the physical phenomena. These are mostly flows, where a large-scale unsteadiness dominates the time-averaged solution. A generic example is a cylinder in crossflow, where steady state solutions do not give an adequate representation of the recirculation zone behind the body. Many technical flows fall into that category, like the highly unsteady flow behind an opening valve in a combustion engine, the unsteady wake developing on the leeward side of buildings, or the strong mixing behind blades and baffles inside stirred chemical reactors. Another prominent example is the flow in a combustion chamber of a gas turbine, which can exhibit a strong vortical instability, which determines the flow topology.
* Category II: Flows, where the steady-state results do not provide the level of detail required for further analysis, even if the time averaged solutions would be sufficiently accurate. Examples are acoustics simulations, where the unsteady flow field is required for an accurate prediction of the noise sources transferred to an acoustics code. Another example is fluid-structure interaction, where in some cases it is necessary to know the unsteady forces in order to determine the dynamical response of the structure. A further challenging problem is the simulation of cavitating flows, where cavitation takes place in the vortex cores of large turbulent structures. Many more such examples could be listed.

Historically, the hierarchy of turbulence modeling methodologies available in CFD codes was Reynolds Averaged Navier-Stokes (RANS), Unsteady RANS (URANS) and Large Eddy Simulation (LES). Flows which could not be computed in steady mode, had to be based on either URANS or LES. Both methods impose severe limitations on the achievable accuracy, partly as a result of the methodology and partly due to the require computing resources. While URANS is sometimes successful (Iaccarino and Durbin, 2000), the results are often unphysical, as URANS tends to provide solutions with one dominating mode, whereas the experiments show a spectrum of scales (Spalart, 2000). The resulting URANS solutions are then of limited use for the two categories described above, as they will neither result in a significant accuracy improvement, when the URANS solutions are time-averaged, nor will they provide the desired detail of the unsteadiness for further analysis.

While LES avoids the limitations of URANS, it imposes severe demands on the computing power, particularly for wall-bounded flows. Despite the substantial investment in LES, is has had little impact on technical flows. The reason is that most technical flows involve wall boundary layers at moderate to high Reynolds numbers, which cannot accurately be handled by LES on current (and foreseeable) computing power, Spalart et al. (1997), Spalart (2000). Hybrid RANS/LES model developments (e.g. Davidson and Dahlström 2005), which combine LES (away from the wall) with RANS (close to the wall), are expected to reduce these limitations in the future. However, these methods are at an early stage of development and will still require substantially more computing power than RANS models for boundary layers.

The combination of RANS and LES into the concept of DES by Spalart (2000), was the first practical approach, which allowed a successful simulation of unsteady technical flows with high Reynolds number boundary layers. The method is based on the idea of using proven RANS models in attached (and mildly separated) boundary layers, while

resolving some of the turbulent scales in large, detached flow regions by an LES method. Numerous successful applications of this method have been reported for different industrial applications (e.g. Squires, 2004). However, there are several open questions and practical concerns in applying DES to industrial flows. DES at current state requires substantial know-how on turbulence modeling and a particular attention to grid generation, much beyond other methods (Spalart, 2001). The essential concern with DES is that it does not continuously change from RANS to LES under grid refinement. In order for LES structures to appear, the grid spacing and time step have to be refined beyond a case-dependent critical limit. In addition, a sufficiently large instability mechanism has to be present to allow the rapid formation of turbulent structures in regions where the DES limiter is activated. If one of the two, or both requirements are violated, the resulting model is undefined and the outcome is largely unpredictable.

Another, recently developed method for unsteady simulations is called Scale-Adaptive Simulation (SAS). It involves the introduction of the von Karman similarity length scale, L_{vK}, into the turbulence model. L_{vK} allows the model to adjust to resolved scales in a simulation. SAS is an improved URANS approach, which avoids the occurrence of unphysical single-mode unsteady flow features, as observed in classical URANS methods. As a result, unsteady regions display a breakdown of the large turbulent structures to smaller and smaller scales as typical for turbulent flows. The method by itself distinguishes between stable and unstable regions of the flow. In stable regions, the model operates in classical RANS mode, whereas in unstable regions, the model displays a LES-like behavior. As the SAS model formulation dos not involve the grid spacing, it avoids the undefined model regimes of DES. In case of overly coarse grids or too large time steps, the model reverts back to the underlying RANS formulation. On the downside, the user has no influence on the "decision" of the SAS model concerning stable vs. unstable regions.

Model Formulations

The central idea behind RANS turbulence models is that two independent scales are required as minimum information for describing the statistical effects of turbulence. This argument is manifested in the formulation of two-equation models, which are solved for two mechanical variables, which can then be used for calculating any other desired mechanical quantity (e.g. length- and time scale). As all transport equation-based RANS models can be viewed as either a simplification (Menter, 1997) or an extension of two-equation models, this principle idea is present in all current RANS models. Considering two-equation models as a black-box, which obtains input from the momentum equations in form of the velocity field, and produces as output two turbulence quantities (and the related eddy viscosity) one would naively assume that two independent scales would have to be provided as input to the source terms in order to allow the models to calculate two output scales. Historically, this was not the case and the source terms only obtain information with dimension [1/time] via the strain-rate and the vorticity tensor. From the source terms, standard RANS models can therefore only determine a turbulence frequency scale, ω. The length scale is a result of the diffusion terms and the boundary conditions (Menter and Egorov 2004). The length scale resulting from standard RANS models is therefore

proportional to the thickness of the turbulent layer, δ, (or the initial/inlet conditions).

Historically, the only RANS model, which has used two independent input scales was the k-kL model of Rotta (1972). This model is based on the formulation of an exact integral length scale, L, and a corresponding exact transport equation for kL. The evaluation of this equation has led to the introduction of the third derivative of the velocity field. This is tantamount to providing an external length scale from the velocity field (assuming a shear layer in y-direction):

$$L_{Rotta} = c \sqrt{\left|\frac{\partial U}{\partial y}\right| \bigg/ \left|\frac{\partial^3 U}{\partial y^3}\right|} \qquad (1)$$

For practical reasons, this formulation was never used in any implementation of the kL model, and the provision of an external length scale remained an episode in turbulence modeling.

A higher derivative appeared later in the KE1E model (Menter, 1997), which is based on a transformation of the k-ε model to a one-equation eddy-viscosity model, assuming equilibrium conditions ($P_k = \rho\varepsilon$). The resulting model was (in its basic form):

$$\frac{\partial(\rho v_t)}{\partial t} + \frac{\partial(\rho U_j v_t)}{\partial x_j} = c_1 \mu_t S - \tilde{c}_2 \rho \left(\frac{v_t}{L_{vK}}\right)^2 + \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma}\frac{\partial v_t}{\partial x_j}\right) \quad (2)$$

where S is the strain rate, v_t is the eddy-viscosity and L_{vK} is the von Karman length scale:

$$L_{vK} = \kappa \left|\frac{\partial U_1/\partial x_2}{\partial^2 U_1/\partial x_2^2}\right| \qquad (3)$$

It is interesting to note that the term containing L_{vK} appears from the transformation of the diffusion terms of the $k-\varepsilon$ model, supporting the above argument that in standard two-equation models, the diffusion terms determine the turbulent length scale. The KE1E model shows a remarkable behavior when solved in unsteady mode for a cylinder in cross-flow (or other unsteady flows). It deviates from the underlying two-equation k-ε model by allowing a LES-like resolution of the otherwise single-mode URANS instability. This behavior of the KE1E model was termed Scale-Adaptive Simulation (SAS), as it allows the model to operate in RANS and LES-like mode, depending on the flow situation. As the transformation resulting in the formulation of the KE1E model did not provide any additional physical information, the appearance of L_{vK} and the corresponding SAS behavior of the KE1E model are largely a coincidence.

In order to arrive at a more physical foundation of SAS, Menter and Egorov (2004) re-visited Rotta's length-scale equation. It was found that some of the arguments used in the derivation of the k-kL model have been overly restrictive (homogenous, isotropic turbulence) and that the leading term in Rotta's expansion should contain the second velocity derivative instead of the third derivative. The resulting model formulation is as follows (reformulated as a $\sqrt{k}L \sim v_t$ model):

$$\frac{\partial k}{\partial t} + U_j\frac{\partial k}{\partial x_j} = P_k - c_\mu^{3/4}\frac{k^2}{\Phi} + \frac{\partial}{\partial x_j}\left[\frac{v_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right]$$

$$\frac{\partial \Phi}{\partial t} + U_j\frac{\partial \Phi}{\partial x_j} = \zeta_1\frac{\Phi}{k}P_k - \hat{\zeta}_2 v_t S|U''|\frac{\Phi^2}{k^{3/2}} - \zeta_3 \cdot k + \frac{\partial}{\partial x_j}\left[\frac{v_t}{\sigma_\Phi}\frac{\partial \Phi}{\partial x_j}\right]$$

$$v_t = c_\mu^{1/4}\Phi \; ; \qquad (4)$$

$$\hat{\zeta}_2 = \zeta_2 \max\left(c_{SAS}; \left|\frac{L'}{\kappa}\right|\right)$$

$$|L'| = \sqrt{\frac{\partial L}{\partial x_j}\frac{\partial L}{\partial x_j}}; \quad |U''| = \sqrt{\frac{\partial^2 U_i}{\partial x_j \partial x_j}\frac{\partial^2 U_i}{\partial x_k \partial x_k}}; \quad P_k = \nu_t S^2$$

with the constants:

ζ_1	ζ_2	ζ_3	σ_k	$\sigma_\Box$	c_μ
0.8	3.51	0.0329	2/3	2/3	0.09

c_{SAS} can used for calibrating the "LES" portion of the model (Menter and Egorov, 2004).

The k-ν_t model has also been transformed and adjusted to the SST model by Menter and Egorov (2005), in order to allow the use of SAS in an existing and technically proven two-equation model. The transformation results in an additional term to the ω-equation:

$$F_{SST-SAS} = \rho \cdot F_{SAS} \max \left[\begin{array}{c} \hat{\zeta}_2 \kappa S^2 \dfrac{L}{L_{\nu K}} - \dfrac{2}{\sigma_\Phi} k \cdot \\[2ex] \max\left(\dfrac{1}{\omega^2}\dfrac{\partial \omega}{\partial x_j}\dfrac{\partial \omega}{\partial x_j}, \dfrac{1}{k^2}\dfrac{\partial k}{\partial x_j}\dfrac{\partial k}{\partial x_j}\right), 0 \end{array} \right] \quad (5)$$

where $\hat{\zeta}_2 = \zeta_2 c_{sas}$. F_{SAS} allows the model to be optimized in the framework of the SST model. Values of $F_{SAS}=1.25$ and $c_{sas}=0.5$ are being used.

Flow Solver

All simulations have been carried out with the commercial CFD code CFX-5. It is based on the coupled solver for mass and momentum and uses an algebraic multi-grid algorithm for convergence acceleration. The numerical scheme is a co-located pressure based method for all Mach numbers. The spatial discretisation switches between a second order accurate upwing biased scheme in the RANS region and a second order central scheme in the LES-regions. The switch is the same as described by Strelets (2001). The time integration uses a second order accurate backward Euler formulation.

DISCUSSION

Scale Resolution

The ability of the SAS model to operate in RANS and LES mode is a result of the use of the von Karman length scale $L_{\nu K}$. In RANS flows $L_{\nu K}$ adjusts to the thickness of the shear /boundary layer. In unsteady flows, it adjusts to the size of the resolved structures. Assuming source-term-equilibrium, one obtains an eddy-viscosity in the "LES" region of:

$$\mu_t = \rho(c \cdot L_{\nu K})^2 S \quad (6)$$

where the constant c depends on the specific underlying model formulation. In LES regions, the turbulent structures break down to the grid size ($L_{\nu K} \sim \Delta$), resulting in a classical LES method. The constants in the SAS model are calibrated to provide a LES-like damping in that limit.

Figure 1 shows a cylinder in cross-flow using the SST model, in URANS and in SAS mode. While the URANS model produces a single-mode vortex separation, the SAS model gives a breakdown of the unsteady structures into a turbulent spectrum. The model behaves therefore much like a DES model, but with some important differences as will be discussed later.
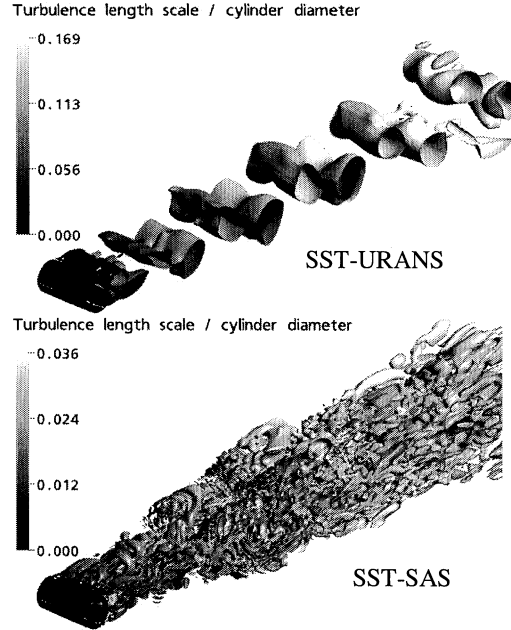

Figure 1: Comparison of SST-URANS and SST-SAS solutions for cylinder in crossflow (Re=3.6×10^6)

The LES-like behavior of the SAS model is best demonstrated for the prediction of the decay of homogenous isotropic turbulence (DHIT). For this test case, a generic divergence-free initial turbulent flow field, based on the experimental spectrum is produced for a cubical domain with a 32^3 and a 64^3 grid. The decay of the turbulent fluctuations depends on the level of eddy-viscosity provided by the turbulence model, as well as on the dissipation of the numerical scheme. The present simulations are carried out using a second-order accurate central difference scheme in space and a second-order backward Euler method in time. Periodic boundary conditions are employed in all three directions. Initial conditions for the turbulence variables are produced by running the turbulence model on the frozen initial velocity field until it reaches steady state. It is important to note that standard two-equation models would not produce such a steady-state initial solution, as no length scale is available to the model.

Figure 2 shows the turbulent spectra of the resolved scales for a non-dimensional time t=0.87 in comparison with LES simulations using the Smagorinsky model and the experimental results of Comte-Bellot (1971). It can be seen that SAS and LES results are virtually identical for both grids. The deviation from the experiments at higher wave numbers is a result of the second order numerics. A higher order discretisation method is currently formulated. The results show that SAS provides a full LES capability, even though no information on the grid spacing is used in the model formulation.
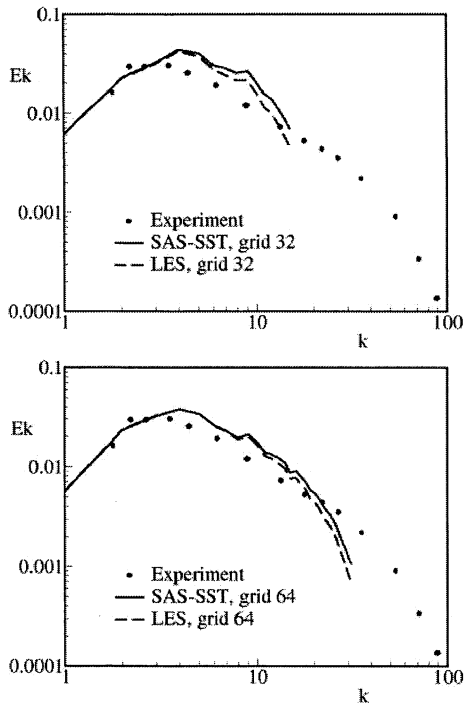
Figure 2: Decaying homogenous isotropic turbulence. Comparison of SAS, LES (cs=0.21) and experiments at non-dimensional time t=0.87. Top: 32^3 grid. Bottom 64^3 grid.

SAS and DES

While SAS and DES provide a similar functionality in principle, there are important practical differences between the two formulations. SAS is essentially an improved URANS formulation, which allows the resolution of the turbulent spectrum in unstable flow conditions. DES on the other hand is the combination of RANS and LES methods. The switch between both is achieved by the comparison of the modeled turbulent length scale and the grid spacing. As the grid spacing enters the DES equations explicitly, DES has a significantly stronger mesh sensitivity than SAS. The main practical problems with DES are that certain requirements have to be satisfied in the switching zone between RANS and LES (Spalart, 2001).

The first requirement is that the flow must develop a strong instability once the LES mode is activated. Otherwise the RANS model is reduced, but the unsteady structures do not develop quickly enough to keep the overall turbulent kinetic energy (resolved + modeled) consistent. Such a situation occurs inside boundary layers or channel/pipe flows, if the grid is refined below a critical level. Once this level is reached, the RANS model is reduced, but in most cases no instability develops quickly enough to compensate for the lowered stresses. In severe cases, this can result in grid-induced-separation, as shown in Menter et al. (2003). For industrial applications this is a practical concern, as standard DES models have a RANS grid limit of $\Delta_{max}>\delta$, where Δ_{max} is the maximal local cell length and δ is the boundary layer thickness. This limit can easily be reached in industrial CFD simulations. Using the "shielded" formulation proposed in

Menter et al. (2003), allows to reduce this limit to $\Delta_{max}\sim0.1x\delta$ which is safer, but does still not eliminate the problem entirely. In addition, the shielding will limit the models ability to operate in LES mode for unsteady internal flows, where the shielding is then active over most of the flow domain.

The second requirement for DES is that the grid spacing in the LES region must immediately be of LES-quality, as otherwise the turbulence model will produce a mix of RANS and LES components (Spalart, 2001, Squires, 2004). A good example is the flow over a backward-facing step. Assume that the grid is of LES-quality behind the step in the main flow plane (x,y) and that the "spanwise" resolution defines the DES limiter, $\Delta_{max}=\Delta_z$. In case that Δ_z is larger than an upper critical limit $\Delta_{max}> \Delta_{RANS}$, the model will operate in RANS mode and produce a steady state solution. In case that Δ_z is lower than a lower critical limit $\Delta_{max}< \Delta_{LES}$, the model will operate in LES mode and develop a flow instability past the step with the correct balance of the stresses. However, if $\Delta_{RANS}>\Delta_{max}>\Delta_{LES}$, the model is undefined, and the solution will be neither RANS nor LES. The most likely scenario is that starting from $\Delta_{max}=\Delta_{RANS}$, refinement will impact the underlying RANS model, without allowing an unsteady solution to develop. As a result, the separation zone will grow much larger than in the experiments. From a certain point of refinement, unsteady structures will develop, but they will not start at the step, but further downstream, where the DES limiter has a stronger influence, again resulting in an overly large separation bubble. With further grid refinement, the unsteadiness will move further upstream and eventually the entire separation zone will be computed in LES mode, when $\Delta_{max}< \Delta_{LES}$ is reached. The situation for $\Delta_{RANS}>\Delta_{max}>\Delta_{LES}$ is shown in Figure 3 where the backward facing step of Jovic and Driver (1994) was computed with the SST-DES model with a grid with only 21 cells in spanwise (2xH - H-step height) direction (the simulation is courtesy of V. Sohm from BMW AG - grid-refined solution produced the correct results). The turbulent structures appear much too late and time-averaged flow reattachment takes place at $L_{reattach}\sim15H$. On the same grid, the SST-SAS model will not produce any unsteadiness and return the standard SST-RANS solution with an app. correct value of $L_{reattach}$. It is the central advantage of the SAS approach that the SAS model always has a RANS fallback position.
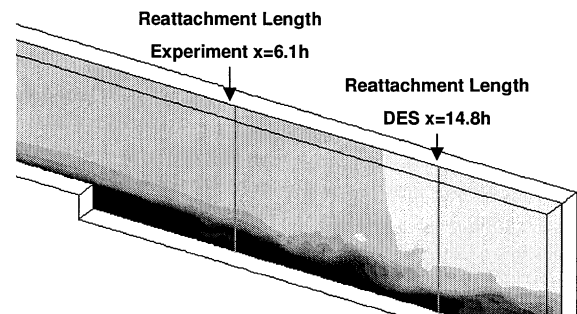

Figure 3: Unsteady flow from DES over backward facing step using insufficient spanwise grid resolution (Courtesy of Sohm from BMW AG)

Steady versus Unsteady Mode

The SAS method is an improved URANS formulation, with the ability to adapt the length scale to resolved turbulent structures. In order for the SAS method to produce a resolved turbulent spectrum, the underlying turbulence model has to go unsteady. This is typically the case for flows with a global instability, as observed for flows with large separation zones, or vortex interactions. There are many technical flows, where steady state solutions cannot be obtained or where the use of smaller time steps results in unsteady solutions. One could argue that the occurrence of unsteady regions in a RANS simulation is the result of a non-local interaction, which cannot be covered by the single-point RANS closure. All these flows will benefit from the SAS methodology.

On the other hand, there are classes of flows, where the SAS model will return a steady solution. The two main classes are attached or mildly separated boundary layers and undisturbed channel/pipe flows. These flows (or areas in a complex flow domains) will be covered by the RANS formulation. This behavior of SAS is ideal for many technical applications, as flows for which the model produces steady solutions are typically those, where a well-calibrated RANS model can produce accurate results. Contrary to DES, SAS cannot be forced to go unsteady by grid refinement. It has been shown however in the backstep simulation above, that enforcing unsteadiness by grid refinement does require an in-depth understanding of the flow, the turbulence model and its interaction with the grid to produce reliable results. Nevertheless, there will be cases, where the grid sensitivity of DES will be advantageous, as it allows unsteady simulations, where SAS might produce a steady state flow-field.

An open question concerns the averaging of the equations. The SAS methodology is derived on RANS arguments, and the appearance of resolved turbulent structures is in contradiction with that averaging concept. This is a general problem with URANS, as URANS is not a defined methodology (Menter et al., 2003). Note that the SST-URANS solution shown in Figure 1 can also not be obtained by any averaging of experimental data, as this solution does physically not exist. From a practical standpoint, the ability of a turbulence model to resolve turbulent structures is only a result of the magnitude of the eddy-viscosity, which is produced by the turbulence model. For the momentum equations, the particular procedure by which the equations have been derived is of secondary nature. Nevertheless, a proper definition of URANS still awaits its inventor.

Flow in a Combustor

The instabilities in gas turbine combustion chambers are of strong technical interest, as they can produce noise and also compromise the structural integrity of the chamber. The unsteadiness can be caused by different mechanisms like flow instabilities introduced by the high swirl in the burner or thermoacoustic instabilities from combustion itself. Even for cold flow conditions, the flow in combustion chambers can be highly unstable and exhibit a strong swirl instability.

The SST-SAS and the SST-DES model were applied to the ITS test-rig with a single burner. This burner was typical for industrial gas turbine combustion systems. The test-rig was built as rectangular combustion chamber. This configuration was investigated experimentally by Schildmacher and Koch (2004). For the evaluation of the models, the test case without combustion was computed. As experimental data are only available in the central part of the chamber, the ITS combustion chamber is mainly a test of the LES-capabilities of the SAS approach. It should be noted however, that in industrial simulations, there is an increasing interest also in the heat transfer through the boundary layers on the chamber walls, or the inlet part to the swirler, which makes a pure LES simulation impractical.

The grid used for the simulations is shown in Figure 4. It consists of 3,600,00 tetrahedral elements, corresponding to 600,000 control volumes of the dual mesh.
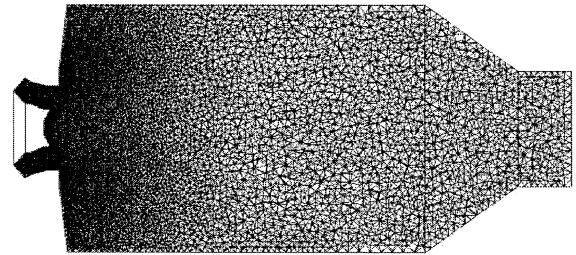

Figure 4: Unstructured mesh for ITS combustion chamber

The flow enters the chamber with a strong swirl component, which is the cause of a swirling instability, requiring an unsteady simulation.
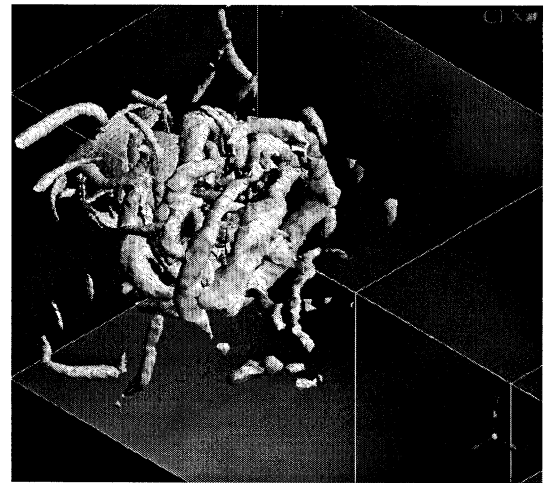

Figure 5: Iso-surfaces of S^2-Ω^2 for ITS combustion chamber computed with SST-SAS model

Figure 6 shows the comparison of profiles for the steady k-ε model, the SST-DES and the SST-SAS model.

The flow topology at a given instance in time is shown in Figure 5 as an iso-surface of S^2-Ω^2. Both, the SST-DES and the SST-SAS model produce significantly better profiles than the steady k-ε model (note that a steady SST model would be virtually identical to k-ε for this free shear flow). As the current flow is mainly an LES test case, there are no strong differences between the SAS and the DES model. The results confirm that SAS is a viable method for such a complex flow.
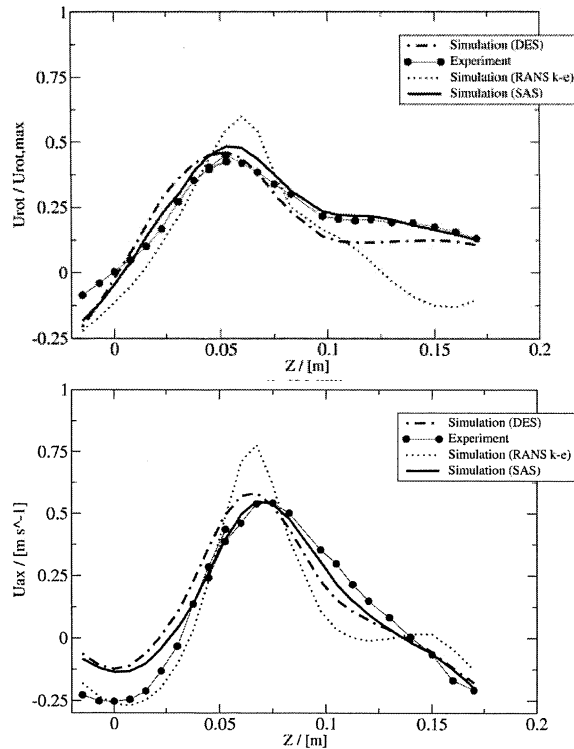
Figure 6: Comparison of averaged velocity profiles from k-ε-, SST-DES and SST-SAS simulations. Top – circumferential velocity at x/D=1.15. Bottom axial velocity at x/D=1.15 (D inlet diameter).

CONCLUSIONS

The concept of Scale-Adaptive Simulation (SAS) has been discussed with an emphasis on the scale-resolving capabilities of the method. It was shown that the SAS model can operate in mixed RANS/LES mode for a cylinder in cross flow. The ability of the model to compute resolved turbulence with the same accuracy as an optimized (adjusted Smagorinsky constant) LES method has been demonstrated for the decaying homogenous isotropic turbulence in a box. Finally, the method was applied successfully to the cold flow in a combustion chamber.

The distinguishing factor of the SAS approach to existing RANS/LES methods is that the model is formulated independent of the grid spacing. The method is therefore an improved URANS formulation. The main practical advantage of SAS is that the explicit grid dependence of the DES method is avoided. It is therefore less grid/user dependent and avoids situations where the DES model is essentially undefined. It is expected that SAS will greatly extend the range of URANS modeling and will have a significant practical impact on industrial flow simulations.

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