Application of Detached Eddy Simulation to Lagrangian Spray Simulations

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Abstract

In this study, the influence of turbulence models on the prediction of turbulent structures is investigated by example of a hollow-cone spray. The focus is put on the general character of the turbulence models, i.e. the production and dissipation of turbulence and the dispersion of the disperse phase. The models in focus include five RANS and LES models, and a Detached Eddy Simulation, which shows LES behavior in the free flow, and falls back to a RANS simulation in regions of small turbulent length scales. Results indicate that Detached Eddy Simulations are less mesh sensitive than true LES, while resolving turbulent features in an LES manner.

Introduction

Lagrangian simulations of liquid sprays involve models for many small scale processes, including primary and secondary breakup or droplet collisions in the liquid phase, and turbulence in the gas phase. For turbulence modelling, two classes of models have evolved: first, turbulence models based on Reynolds Averaging of the Navier Stokes equations (RANS models), second and more recently spatially averaging Large Eddy Simulations (LES). Most common RANS models are k-epsilon- and k-omega-models, which describe turbulence in terms of turbulent kinetic energy and the (specific) turbulent dissipation rate. LES models are distinguished by the subgrid-scale-model for small-scale turbulence. Studies by other authors have shown that the choice of the turbulence model has a major influence on the accuracy of Lagrangian spray simulations.

While most liquid phase models are based on a RANS description of the gas phase, RANS turbulence models are not capable to capture vortex creation and break down in highly unsteady free jets. In contrast, LES can describe free jet turbulence very well, but does not link to many liquid phase models properly, as it does not provide time-averaged quantities. This trade-off can be overcome by hybrid turbulence models, such as Detached Eddy Simulation (DES). Contrary to classical hybrid LES-RANS models, which decompose the domain into dedicated LES and RANS regions, DES is basically an LES approach with RANS for subgrid-scale-modeling, i.e. the turbulent transport equations are solved for the entire domain. When combined with a k-epsilon-model, DES can provide the turbulent quantities required by the liquid phase models, while maintaining LES behavior in the free flow.

In this study, the application of DES to Lagrangian spray simulations is assessed by example of a hollow-cone spray as found in gasoline direct injection engines. The DES model is coupled to a realizable k-epsilon model, and compared to LES and RANS simulations of the same case (including standard k-epsilon, RNG-k-epsilon and realizable k-epsilon models). For all turbulence models, a mesh sensitivity analysis is performed. The influence of turbulence modeling on the spray simulation is evaluated by macroscopic properties such as liquid penetration, vortices formed etc., and by microscopic properties and turbulent quantities, such as turbulent kinetic energy (for the DES and RANS models), turbulent intensities and dissipation rates.

RANS Models

RANS turbulence models are based on the decomposition of velocities into mean values and temporal fluctuations. While linear fluctuation terms are eliminated by Reynolds Averaging, non-linear fluctuation terms such as Reynolds stresses require modeling. The family of k-epsilon-models describes turbulence by means of turbulent kinetic energy k and turbulent dissipation rate ϵ, which are defined by scalar transport equations:

$$\frac{\partial}{\partial t}\left(\rho k\right) + \frac{\partial}{\partial x_i}\left(\rho k u_i\right) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k - \underbrace{\rho\epsilon}_{D_k} + S_k \tag{1}$$

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$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + \underbrace{C_{1\epsilon}\frac{\epsilon}{k}P_k}_{P_\epsilon} - \underbrace{C_{2\epsilon}\rho\frac{\epsilon^2}{k}}_{D_\epsilon} + S_\epsilon \tag{2}$$

In addition to the convective and diffusive terms common to all scalar transport equations, production terms P and dissipation terms D are found in both equations. The virtual increase of viscosity μ is accounted for by a turbulent viscosity μ_t which is modeled in terms of k and ϵ:

$$\mu_t = \rho\, C_\mu \frac{k^2}{\epsilon} \tag{3}$$

While the dissipation of k is defined by the turbulent dissipation rate ϵ, the production of k is proportional to the strain rate modulus S:

$$P_k = \mu_t S^2 \tag{4}$$

Due to the proportionality of $P_k \sim \mu_t \sim k^2$, the production of k may be self-amplifying if not balanced by turbulent dissipation rate. For all equations, C and σ designate model constants, and S_k and S_ϵ are optional source terms. For compressible or buoyancy driven flows, both equations must be extended by additional production and dissipation terms [1].

Based on the standard k-epsilon-model (STD-model), other k-epsilon-models have been derived, such as the "renormalized group" k-epsilon model (RNG-model) or the "realizable" k-epsilon model (RKE-model). Except for minor differences such as model constants or the formulation of effective viscosity, the major difference between these models is the formulation of the turbulent dissipation rate:

RNG-model: The RNG-theory describes a mathematical method to determine model constants by spectral analysis of turbulent scales. Contrary to the proposal of Taskinen [2], the model constants of the RNG-model are not considered adjustable. However, the main difference between the RNG- and the STD-model is an extension of the ϵ-equation, which increases turbulent dissipation rate in regions of high strain rates, compensating for an over-prediction of turbulent kinetic energy.

RKE-model: In the context of k-epsilon-models, "realizability" means tha tthe model holds specific mathematical restrictions, i.e. turbulent quantities cannot become non-physical by mathematical issues only. The RNG- and STD-models are "non-realizable", as for example the production and dissipation terms P_ϵ and D_ϵ given in Eq. 2 form singularities for $k = 0$. The RKE-model proposed by Shih et al. [3] is considered "realizable" and has been validated for a wide range of flows [3, 4].

Large Eddy Simulation

Contrary to RANS simulations, LES is not based on temporal averaging of fluctuation terms, but on spatial filtering, which is achieved implicitly by spatial discretization. By that, LES is capable to resolve temporal fluctuations, while losing spatial information below grid scale. The effect of such small-scale turbulence must be described by adequate subgrid-scale models (SGS-models):

Smagorinsky-Lilly: The Smagorinsky-Lilly SGS-model describes turbulent viscosity in terms of resolved local shear stresses and mixing lengths, which are defined by cell dimensions in the context of LES [1]. When referring to LES in this paper without further specification, the Smagorinsky-Lilly SGS-model is meant.

Kinetic-Energy-Transport: While the Smagorinsky-Lilly SGS-model expresses turbulent viscosity directly by resolved shear stresses, the Kinetic-Energy-Transport model (TKE-LES-model) introduces a subgrid turbulent kinetic energy, which is defined by a transport equation similar to the k-epsilon RANS-models. The difference is that dissipation of turbulent kinetic energy is not described in terms of a turbulent dissipation rate, but depends on local resolution only, i.e. on cell dimensions [4, 5]. The TKE-LES-model is introduced here due to its similarity to k-epsilon-based Detached Eddy Simulations.

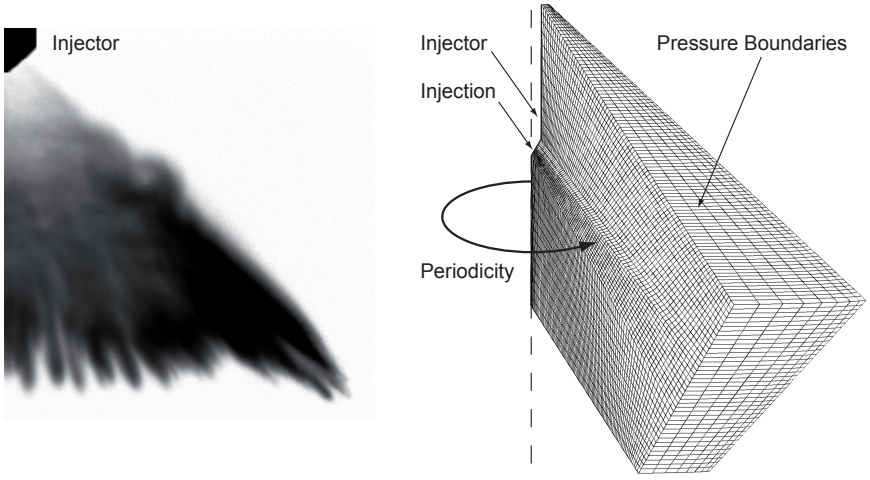

Figure 1: Photography of the hollow-cone spray and schematic of the coarse mesh. For efficiency reasons, a 45° segment is simulated. Periodicity is considered by adequate boundary conditions. The pressure boundaries do not enforce any free flow.

Detached Eddy Simulation

Initially, DES was proposed to deal with high-resolution requirements of LES in boundary layers. Starting from a RANS model, the DES approach limits turbulent lengths scales to grid resolution, modeling small-scale turbulence while resolving large-scale turbulence in an LES manner. While initially coupled to the Spalart-Almeras turbulence model not introduced here [6], it was later applied to k-omega-based models successfully [7, 8].

In this study, a RKE-based DES model is shown, which is proprietary to the commercial CFD-code ANSYS FLUENT [5]. The DES character is introduced in the k-equation and in the formulation of turbulent viscosity μ_t by substitution of the turbulent length scale

$$\frac{k^{3/2}}{\epsilon} \rightarrow l_{\mathrm{des}} \tag{5}$$

and elimination of ϵ. For Eq. 1, this is

$$\frac{\partial}{\partial t}\left(\rho k\right) + \frac{\partial}{\partial x_i}\left(\rho k u_i\right) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k - \underbrace{\rho\frac{k^{3/2}}{l_{\mathrm{des}}}}_{D_k} + S_k \tag{6}$$

The length scale l_{des} is the minimum of either the turbulent length scale as given by the RKE model, or the maximum cell dimension Δ,

$$l_{\mathrm{des}} = \min\left(\frac{k^{3/2}}{\epsilon}, C_{\mathrm{des}}\Delta\right) \tag{7}$$

where C_{des} is a model constant. For small turbulent length scales, Eq. 6 returns to its RANS equivalent as given in Eq. 1. For large turbulent length scales, dissipation of turbulent kinetic energy is attributed to subgrid-scale turbulence, resolving large-scale turbulence similar to the TKE-LES-model instead of dumping it into turbulent kinetic energy. Consistently, by limiting turbulent length scales to a maximum of $C_{\mathrm{des}}\Delta$, the dissipation term D_k is deliberately larger than its RANS model equivalent, reducing turbulent kinetic energies when compared to the RKE-model [5]. Therefore, while the turbulent dissipation rate ceases validity in LES-regions, the turbulent kinetic energy is valid across the entire domain.

Case Description

For demonstration, we choose a Lagrangian simulation of a hollow-cone spray under steady-state ambient conditions. Due to its complex turbulent structures, this demonstration case is very sensitive to the

Table 1: Temporal and spatial discretization schemes for all transport equations as applied to RANS, DES and LES simulations.

	RANS			**DES**	**LES**	
	STD	RKE	RNG	RKE	LES	TKE
time	SOI	SOI	SOI	SOI	SOI	SOI
pressure interpolation	PRESTO	PRESTO	PRESTO	PRESTO	PRESTO	PRESTO
pressure momentum	PISO	PISO	PISO	PISO	PISO	PISO
momentum	LU	LU	LU	CD	CD	CD
k	U	LU	LU	LU	–	LU
ϵ	U	LU	LU	LU	–	–
species	LU	LU	LU	CD	CD	CD
energy	LU	LU	LU	LU	LU	LU

SOI: second order implicit, U: (first order) upwind, LU: linear (second order) upwind, CD: central differencing
PISO: pressure implicit by splitting of operators, PRESTO: pressure staggered option

choice of the turbulence model for two reasons. First, the turbulence model dominates the prediction of the gas-phase flow field; by relative velocities, the gas-phase flow field strongly influences droplet motion, vaporization and breakup. Second, turbulent fluctuations are source to turbulent dispersion of the droplet phase and to droplet collisions.

In spray modeling, k-epsilon-based RANS-models are very popular, as they provide time averaged velocities for calculation of relative velocities, and allow simple access to turbulent fluctuations by definition of the turbulent kinetic energy. Among the RANS-models introduced, the RNG-model has gained major significance because of its low diffusivity [9]. In a study similar to this one, Taskinen [2] has compared the STD- and RNG-model and the influence of model constants. The RKE-model was used recently in very high resolution 2D simulation of a hollow cone spray with good results for various boundary conditions [10]. When coupling LES to Lagrangian spray simulation, obtaining velocity fluctuations and considering turbulent dispersion is one major issue. Nishad et al. [11] have conducted 3D simulations of a similar demonstration case, gaining reasonable results without modeling turbulent dispersion at all. The application of DES to spray simulations possibly allows to harvest the benefits of both LES and RANS simulations, i.e. resolving large-scale turbulence while preserving information on velocity fluctuations.

In this study, the gas phase simulation is carried out with ANSYS FLUENT (12.0.16), while the disperse phase is ran on user-implementations of all models involved as presented in earlier 2D and 3D studies [10, 12]. Primary breakup is modeled by a fixed distribution function. Secondary breakup is disabled to avoid any indirect dependencies caused by interaction of the breakup model with the surrounding gas phase. Vaporization is described by a discrete multi-component model as proposed by Sirignano [13]. The collision algorithm and model are independent of the gas phase mesh, using an anisotropic Lagrangian collision algorithm [12].

Numerics

The simulation is carried out on a 45° segment of the hollow cone spray. To investigate mesh sensitivity, three similarly structured meshs are introduced (fine: 200k cells, intermediate: 100k cells, coarse: 30k cells, Figure 1). Temporal resolution is held constant at time-steps of 1 µs. The momentum equations are solved with a segregated pressure-based solver. Unless stated differently, spatial discretization of convective terms is second order upwind. For the STD-model, the k- and ϵ-equations are resolved with a first order upwind scheme to address stability. For DES and LES, species and momentum are discretized with central differencing schemes, while turbulent quantities are resolved by upwind schemes as before. To reduce overshoots at face values, a minmod slope limiter is applied to all upwind schemes. Pressure-momentum coupling is achieved with a pressure-implicit method (PISO), running a staggered-grid interpolation on the pressure field (PRESTO) proprietary to ANSYS FLUENT [5]. Temporal discretization is second order implicit for all cases. An overview over numerical settings is given in Table 1.

Results

The intention of this study is to show the hybrid character of DES and its behavior in Lagrangian spray simulations. Therefore, except for Figure 1, which gives a general impression of the expected spray shape, no experimental results are shown; the focus is put on model comparisons instead.

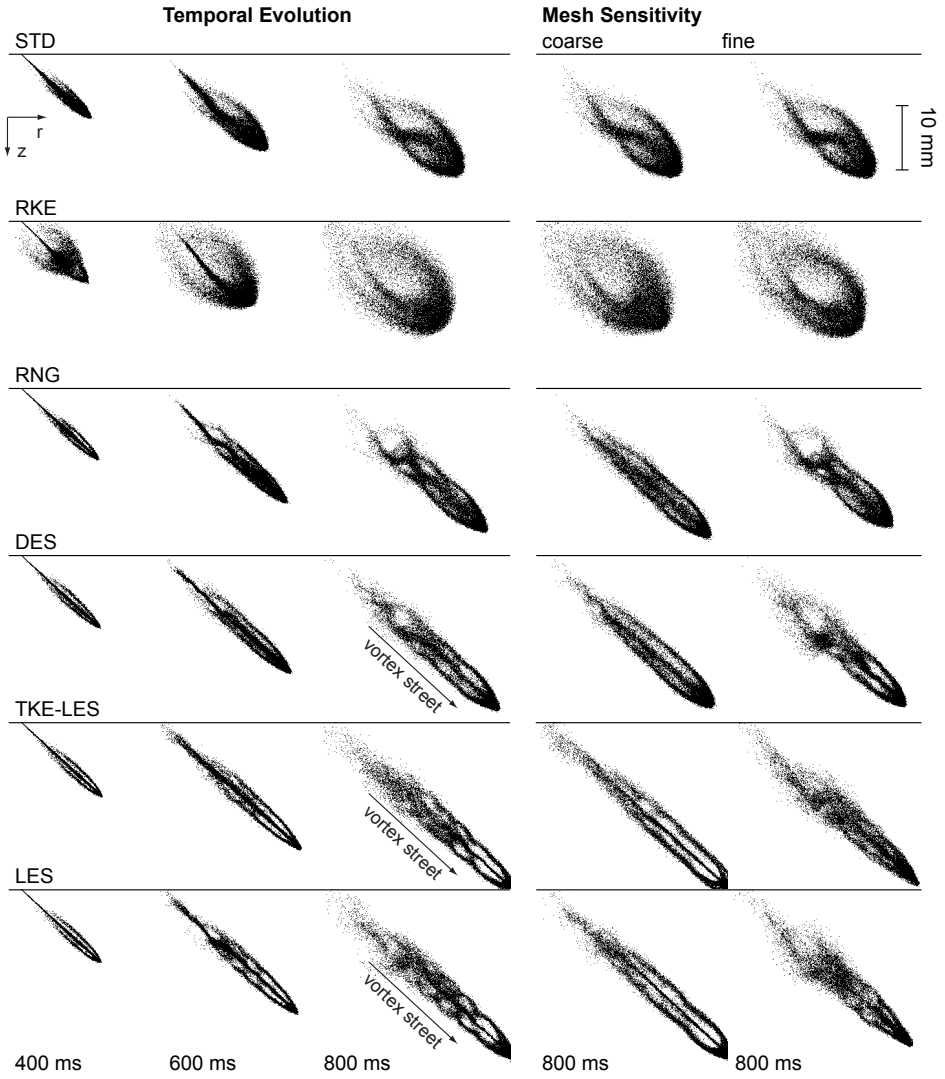

Figure 2: Droplet positions over time (intermediate mesh, left) and for differently resolved meshes (right). The STD- and RKE- models are overly dispersive. The other models predict similar spray shapes, differing in the resolution of turbulent features and in mesh sensitivity.

Macroscopic Quantities

Generally, the choice of the turbulence model has a major influence on droplet motion and dispersion. Figure 2 shows droplet positions for three time steps after start of injection, and a mesh sensitivity analysis. With the STD- and RKE-models, turbulent dispersion is heavily over-predicted, leading to very short penetration and diffuse vortex positions. While the overly diffusive behavior of the STD-model is known from other publications [2, 9], the poor performance of the RKE-model is surprising, as simulations on a very fine mesh (100k cells, 2D) have lead to promising results [10]. In agreement to the findings of Taskinen [2], the RNG-model resolves vortex structures properly, showing some loss of detail for the coarse mesh, and no significant mesh influence for the fine mesh.

The LES-models show very similar behavior each, resolving a vortex street along the direction of penetration, which is not visible with either RANS-model. However, visible mesh dependencies are significant, leading to a loss of information for the coarse mesh and a more dispersed spray shape for the fine mesh. Considering that LES is based on spatial filtering and thus inherently mesh-dependent, this finding is not unexpected.

The DES combines the properties of LES- and RANS-models. While the DES simulation resolves turbulent features similarly to the LES simulations, the mesh-independence is nearly up par to the RNG-model, which is the best performing RANS-model investigated. The good results obtained from the DES

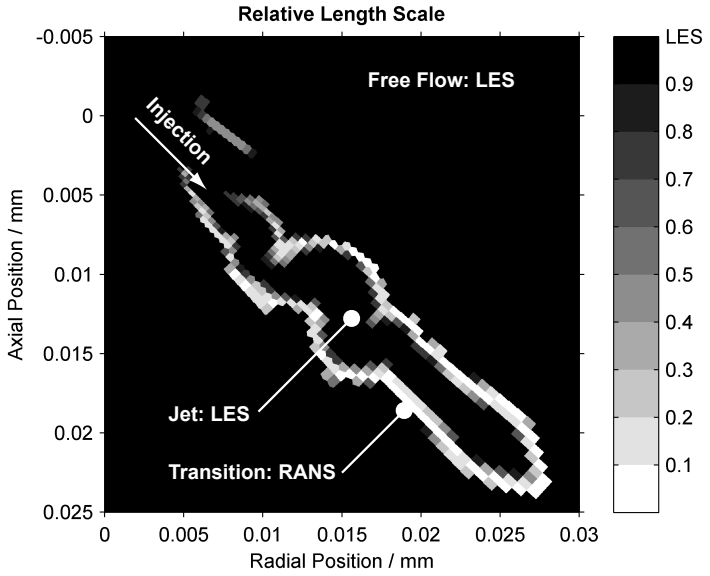

Figure 3: Relative DES length scale $l_{\mathrm{des}}/C_{\mathrm{des}}\Delta$ at the end of the simulation (800 µs). A value of 1 indicates LES behavior, where dissipation of turbulent kinetic energy is defined by cell length scales. Except for the transition regions between the jet and the free flow, LES behavior is predominant.

raise some questions on the RKE-model which it is based on, and which is a poor performer in its RANS implementation. As the DES substitutes the turbulent dissipation rate by local length scales over most of the domain as shown in Figure 3, the formulation of the turbulent dissipation rate must be the source to the overly diffusive results obtained from the RANS simulation.

Numerically, DES, LES, and the RNG-model do not show any stability issues. However, for DES and LES, the central differencing discretization leads to significant checkerboarding artifacts in regions of high velocity gradients as found near the point of injection. This issue can be addressed by switching to a bounded central differencing scheme, which fades into upwind schemes in regions were oscillations may occur. However, as the upwind bias of bounded central differencing has lead to significant damping of vortex structures in preliminary investigations, the use of this differencing scheme is not advised.

Turbulent Quantities

To understand the reasons for the different results obtained, mean turbulent quantities are evaluated for the RANS- and DES-models, i.e. the mean turbulent intensity $\bar{I}$ and the mean turbulent time-scale $\bar{\tau}$:

$$\bar{I} = 2\frac{\int \rho k \, dV}{\int \rho v^2 \, dV} \qquad \text{and} \qquad \bar{\tau} = \frac{\int \rho k \, dV}{\int \rho \epsilon \, dV} \tag{8}$$

These quantities are nearly independent of the domain size, as any additional void volume does not contribute to either k, ϵ, or v^2. Figure 4 (top) shows that the poor performing STD- and RKE-models are designated by high turbulent intensities, and in the case of the RKE-model of a large turbulent time-scale leading to slow dissipation of turbulent kinetic energy. The reason for the high turbulent intensity is not only found in the ratio of production and dissipation of turbulent kinetic energy as shown in Figure 4 (bottom), but rather in the early onset of turbulent production, which may be caused by local self-amplification as discussed with Eq. 4.

For turbulent intensities, Figure 5 shows a mesh sensitivity analysis. At early stages of injection, near-nozzle velocity gradients are resolved by one cell distance only, reconstructing steeper gradients if the mesh is refined. As the production of turbulent kinetic energy is directly proportional to local velocity gradients, mesh refinement leads to a growth of turbulent intensities. While the STD- and RNG-models show significant mesh dependencies at early stages of injection only, the RKE-model maintains mesh dependencies throughout the simulation, which is not desirable for a RANS-model. For the DES-model, mesh refinement means that more turbulent scales are resolved, and less turbulent scales are modeled. The decrease of turbulent intensities for refined meshes is expected; however, it is unclear which part of

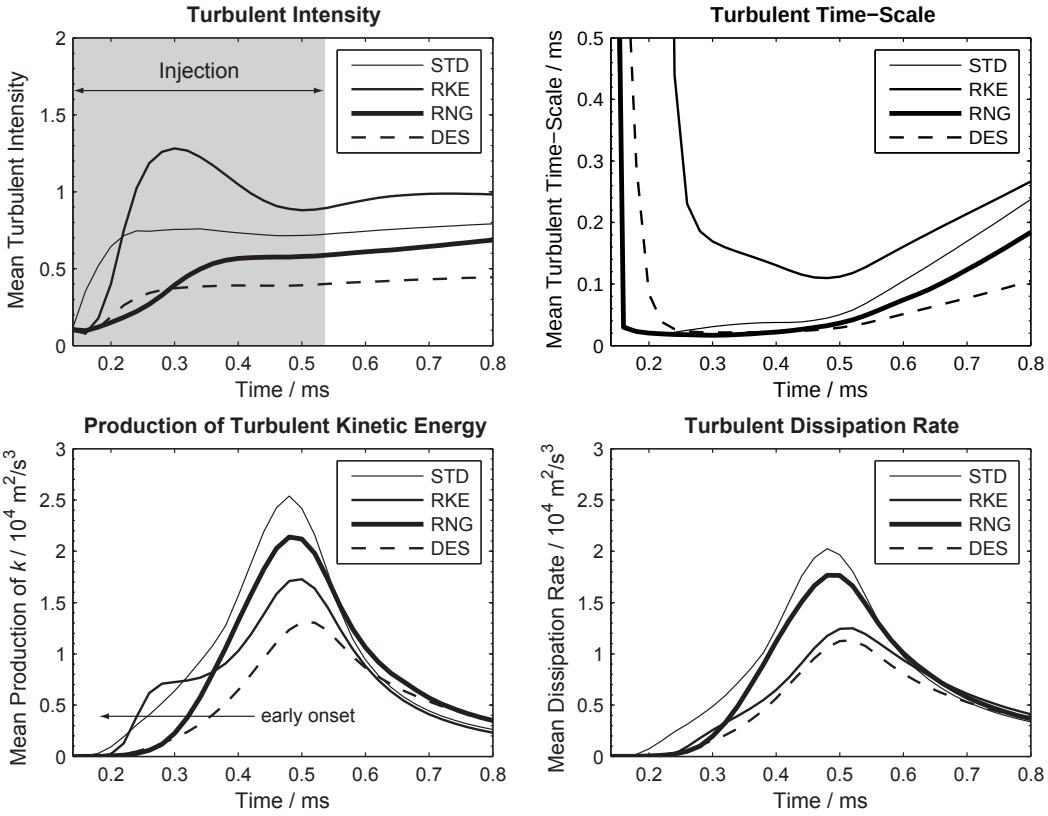

Figure 4: Turbulent quantities for the intermediate mesh. Model dependencies originate from different production/dissipation ratios of turbulent kinetic energy, leading to different turbulent intensities and time-scales.

the mesh dependencies must be attributed to the character of the DES-model, and which part must be considered a true mesh dependency to be led back to the underlying RKE-model.

Conclusions

In this study, a Detached Eddy Simulation was compared to LES and RANS models. Results indicate that DES can handle free jet turbulence similar to true LES models. The DES approach shows low diffusivity of turbulent quantities, and turbulent dissipation is reduced. This is remarkable when compared to the RKE-RANS-simulation it is based on, which has shown overly diffusive behavior. For the spray simulation, the reduced diffusivity leads to increased liquid phase penetration in comparison to RANS simulations, and to a more distinct prediction of turbulent structures, which are dissipated by RANS models to great extent.

In contrast to the LES simulations, turbulent fluctuations can be derived from turbulent kinetic energy, and used for the prediction of turbulent dispersion. The dispersion model is crucial to the formation of droplet recirculation regions, which is a known issue when coupling Lagrangian spray simulations to LES simulations. As assumed, the DES simulation appears to combine beneficial properties of LES and RANS simulations.

Future studies should focus on three key issues: First, a mesh-independent formulation for the near-nozzle production of turbulent kinetic energy must be found to reduce mesh dependencies in RANS- and DES-models, e.g. by applying the jet theory proposed by Abani et al. [14]. Second, DES-implementations involving the RNG-model should be tested thoroughly, which appears to be the reference RANS-model for spray simulations, and remaining mesh dependencies must be reduced. Finally – despite the good results – the combination of DES with Lagrangian spray simulations requires further validation by synthetic test cases for classical applications, such as in-cylinder simulations. For latter, where boundary layers and free turbulent structures are of similar importance, DES may play all its benefits.

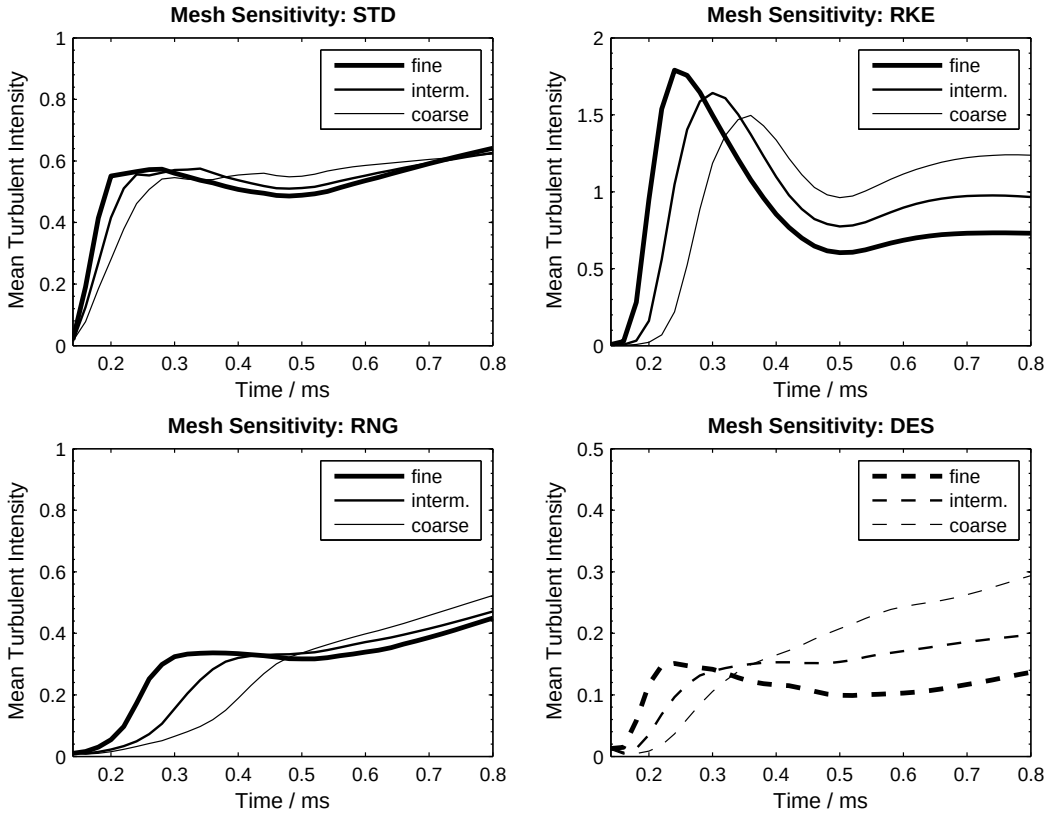

Figure 5: Mesh sensitivity of turbulent intensities. Mesh dependencies originate from early-stage dependencies in the production of turbulent kinetic energy.

Acknowledgments
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