COMPUTATION OF MIXING PROCESSES RELATED TO EGR

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ABSTRACT

Turbulent mixing processes related to the application of exhaust gas recirculation (EGR) in internal combustion engines are investigated using different turbulence models, i.e. RANS and LES. First, the mixing process in a simplified geometry, a T-junction with circular cross-sections, is considered under steady and pulsating in-flow conditions. The focus lies on the evaluation of the applied models and their effect on the mixing under the given flow conditions. The same turbulence models are then applied to a Diesel engine inlet manifold. It is shown that the EGR distribution to the different cylinders is non-uniform and hence affecting the total emissions from the engine. The non-uniformity of the EGR concentration implies also that the smoothing effect of the URANS model may not be adequate for determining the local temporal- and spatial-EGR distribution at the cylinder intakes.

Introduction

Mixing processes in turbulent flows are of high importance in numerous technical applications. Some examples are the mixing of air and fuel in gas turbines or internal combustion engines, mixing of hot and cold water in power plant application and chemical applications, where the mixing quality is an important factor for the rates of chemical reactions, etc. This study aims on the investigation of mixing processes occurring in Exhaust Gas Recirculation (EGR) applications in internal combustion engines (ICE). The basic principle of EGR is to feed-back a portion of the exhaust gas and mix it with the intake air. This results in a dramatical decrease in NOx-emissions, since the lower oxygen concentration of the air/exhaust mixture leads to lower peak temperatures during the combustion process.

There may be some problems when applying EGR due to incomplete mixing. An inhomogeneous mixture of air and EGR among and inside the cylinders might lead to incomplete combustion and soot formation, with too much EGR, and high NOx emissions, with too little EGR.

The goal of this study is to perform a systematical analysis of mixing models, i.e. RANS and LES, under stationary and pulsating in-flow conditions. First, the flow in a T-junction with circular cross-sections is considered. For this case we are able to compare the computational results with available experimental data. Finally, the turbulent mixing models are applied to a Scania Diesel engine manifold.

The general approach to the computation of mixing processes is to compute the flow by solving the Navier-Stokes equation. Because of the high Reynolds numbers occurring in engine applications two methods are currently feasible: Steady and time-dependent Reynolds averaged Navier-Stokes (RANS/URANS) computations and Large Eddy Simulations (LES). In both modeling approaches, the mixing is handled by solving an additional transport equation for the concentration of the EGR.

Mixing of a passive scalar in T-junctions under stationary flow conditions have been investigated in numerous computational and experimental studies. A good overview of the available literature is given in [Hu & Kazimi (2006)]. Recently, mixing predictions with RANS-models have been investigated by [Walker *et al.* (2010)]. It was shown that the mixing predictions with RANS are strongly dependent on the parameters of the scalar model, which are not universal for different flow and geometrical conditions. LES has been applied among others by [Hu & Kazimi (2006)],[Kuczaj *et al.* (2010)] and [Westin *et al.* (2008)]. LES was shown to be a promising approach for the predictions of turbulent mixing. In all previous studies, it was concluded that very high mesh resolutions are necessary for accurate predictions of the scalar quantity. LES has also been applied to the T-junction case in a previous study [Sakowitz & Fuchs (2011)], where the sensitivity to mesh and boundary conditions was analyzed and the governing mixing mechanisms were studied.

Very little literature is available about mixing scalars under pulsating in-flow conditions. Recently, there has been some work on the computation of EGR mixing by [Karthikeyan *et al.* (2011)], where the impact of different geometrical parameters on the mixing was studied. There is, however, no direct evaluation of different approaches under pulsatile flow conditions.

Methods

For the computation and analysis of flows with temperature gradients and high speeds as they occur in combustion engines, the compressible Navier-Stokes equations are solved using the PIMPLE pressure correction method, which is a combination of the SIMPLE and PISO methods. The equations are discretized using central differences of second order in space and an implicit Euler method in time.
The mixing process is modeled by a passive scalar. A passive scalar is a transported quantity that is governed by advection and diffusion only and has no effect on the flow field.
The equation for the passive scalar ϕ has the following form

$$\frac{\partial\phi}{\partial t}+u_i\frac{\partial\phi}{\partial x_i}=\kappa\frac{\partial^2\phi}{\partial x_i^2}, \tag{1}$$

where κ is the molecular diffusivity. By introducing the Schmidt number $Sc=\frac{\nu}{\kappa}$ the equation can be rewritten:

$$\frac{\partial\phi}{\partial t}+u_i\frac{\partial\phi}{\partial x_i}=\frac{\nu}{Sc}\frac{\partial^2\phi}{\partial x_i^2} \tag{2}$$

Applying Reynolds averaging to the equation yields:

$$\frac{\partial\overline{\phi}}{\partial t}+\overline{u}_i\frac{\partial\overline{\phi}}{\partial x_i}=\frac{\nu}{Sc}\frac{\partial^2\overline{\phi}}{\partial x_i^2}-\frac{\partial\overline{u_i'\phi'}}{\partial x_i} \tag{3}$$

In the RANS framework, the last term in equation 3, which is commonly called the turbulent flux vector, has to be modeled. A simple gradient-diffusion model (GDM) is used stating:

$$\overline{u_i'\phi'}=-\frac{\nu_t}{Sc_t}\frac{\partial^2\overline{\phi}}{\partial x_i^2} \tag{4}$$

where ν_t is the turbulent viscosity computed by the turbulence model. For the $k-\varepsilon$ model, used in this study, it is $\nu_t=0.09\frac{k^2}{\varepsilon}$. Sc_t is the turbulent Schmidt number. An empirical value commonly used is $Sc_t=0.7$.
The RANS computations are evaluated by corresponding LES computations. The principal idea of LES is to resolve the large energy-carrying scales and to model the smaller unresolved scales (see for example [Pope (2008)]). The underlying idea is that the smaller scales are more universal and independent of boundaries and can therefore be modeled more easily. In fact one is not interested in the correct behavior of the small scales but only their effect on the large scales, which basically consists of dissipation of turbulent kinetic energy. The applied second order discretization schemes clearly have a dissipative behavior, i.e. the numerics and the modeling of the subgrid scales are interacting. Following this logic, the dissipative effect of the small-scales can be modeled implicitly by using dissipative schemes. This approach is commonly called *Implicit LES*.

Mesh	**cell size**	**total cell amount**
Mesh 1	0.03 D	850,752
Mesh 2	0.015 D	5,144,778

Table 1. Meshes used for the T-junction

Meshes

The meshes used during this study are all hexahedral and uniform. For the case of the T-junction, the mesh sensitivity was assessed for LES and resulted in a quite high demand on the mesh resolution, i.e. mesh 2 in table 1 was used [Sakowitz & Fuchs (2011)]. For RANS mesh 1 in table 1 was found to give suffcently mesh independent results. For the inlet manifold a uniform, hexahedral mesh wit a cell size of 3 mm was used, resulting in approx. 800.000 cells.

The T-junction in stationary flow

The considered geometry equals the one used in experiments at the Vattenfall laboratory [Andersson *et al.* (2006)]. The setup used in these experiments is shown in figure 1. The junction consists of two pipes with circular cross-sections; the cross-section area of the main pipe is twice as big as the one of the branch pipe, i.e. if the velocity ratio between the pipes is 1, the mass flow ratio is 2. The fluid used in the experiments was water. The water in the branch pipe was heated in order to get a temperature difference of about $\Delta T=15K$. The Reynolds number based on the main inflow pipe diameter was $Re=0.96\cdot10^6$.
The measurements conducted during these experiments comprise temperature measurement using thermocouples. The temperature data is available at several positions close to the wall. Furthermore the velocity was measured over some cross-sections upstream and downstream of the junction. The data comprises first and second order moments and allows for a detailed validation of the computational methods.
Figure 2 shows the mean velocity profiles over z at $x=2.6D$ computed by RANS and LES compared to experimental data. The LES predictions are very close to the experiment whereas the RANS computation overpredicts the velocity defect right behind the junction. The turbulent kinetic energy profile, computed as $k=\frac{1}{2}\overline{u_i'u_i'}$, is compared at the same position (see Fig. 3). The RANS models overpredict the turbulent kinetic energy produced by the shear layer.
The passive scalar is compared to the measured temperatures along a line along the x-axis close to the bottom wall of the T-junction (see Fig. 4). The temperature is normalized as $T^*=\frac{T-T_{cold}}{\Delta T}$. There is a large discrepancy between RANS and the experiments, whereas LES is in good agreement with the experiment.
The performance of the RANS computations could of course be improved by adjusting Sc_t. The value of Sc_t will, however,

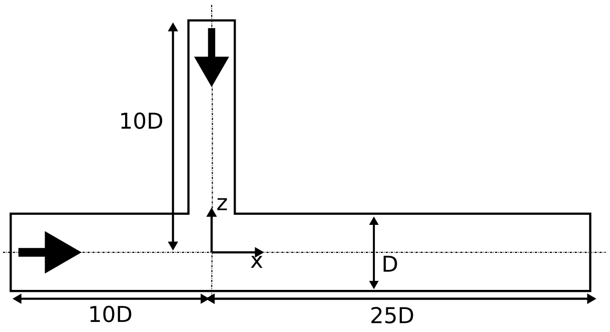

Figure 1. Computational domain (D=0.14m)

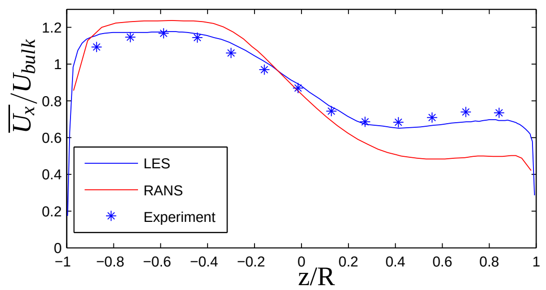

Figure 2. Mean velocity profiles at $x/D = 2.6$

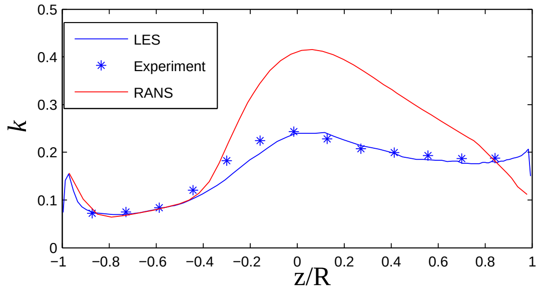

Figure 3. Turbulent kinetic energy at $x/D = 2.6$

always be based on empirical relations and is not universal for different geometries and flows.

The T-junction in pulsating flow

In order to study the influence of incoming pulsations on the mixing process, a time-varying mass flow is specified on the branch inlet. The inlet mass flow is sine-shaped and has an amplitude of 100% of the mean mass flow, i.e. the mass flow on the branch inlet is given by $\dot{m}(t) = \dot{m}_{stat}(1 + \frac{1}{2}sin(2\pi \cdot f \cdot t))$. Two test cases with different pulsation frequencies ($f = 60Hz$ and $f = 300Hz$) were run and are compared in this section. The Strouhal numbers based on the pipe diameter and U_0 are 0.1 and 0.5, resp.

A previous study on this case using LES [Sakowitz & Fuchs (2011)] has shown that there is an instability due to the shear layer that produces velocity fluctuations in z-direction with a frequency of about 300 Hz. When applying a pulsation frequency of 300 Hz this instability is amplified. The flow cannot be described as quasi-stationary because of these resonance effects. As a consequence, these resonance effects cannot be captured by RANS methods. This is illustrated in Figs. 5 and 6 showing the phase average of the z-component of the velocity in a point inside the shear layer for the fluctuation frequencies of 60 Hz and 300 Hz computed by RANS and LES. In the case of 60 Hz LES and RANS are in good agreement. For 300 Hz, one can see that LES predicts much higher fluctuations than RANS, because the resonance effect is not captured by RANS. This is a good example showing the shortcomings of RANS in pulsating flow, when the pulsations interact with the turbulent scales.

Figs. 7 and 8 show the corresponding scalar fluctuations. One can see that RANS and LES agree for the 60 Hz case but not for the 300 Hz case as a consequence of the deviations in the velocity fluctuations. The RANS model works, however, better in pulsating flow than in stationary flow, because the scalar is governed by large scale motions of the fluctuations rather than by the small scales of turbulence.

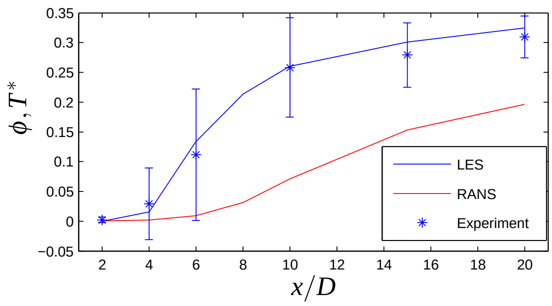

Figure 4. Mean passive scalar and normalized temperature along the x- axis close to the bottom wall, including the RMS of the scalar fluctuations (bars)

The Scania manifold

The methods are now applied to a realistic geometry, i.e. a inlet manifold of a 6-cylinder Scania engine (see Fig. 9). The geometry has two inlets, one for the intake air and one for the recirculated exhausts. Upstream of the EGR inlet there are two bends, that are thought to have an important effect on the flow downstream. The mixture of air and exhaust gases (EGR) are then lead to the cylinders, that are opening and closing according to the cylinder timings. The correct boundary conditions for the flow in real engine operation are unknown and hard to determine. The opening and closing of the cylinders is causing a flow into the cylinder which is determined by the pressure difference between the inlet manifold and the cylinder. This pressure difference is, however, changing in time due to the motion of the cylinder. At the air inlet a stationary inflow can assumed. The EGR flow, however, must be assumed to be pulsating, because the pulsations are transferred from the exhaust valves. In some cases the EGR is cooled down in a EGR cooler, which might decrease the pulsations. The pulsations and flows to the cylinder can be estimated using one-dimensional methods, such as GT-Power. These one-dimensional computations have, however, fairly high uncertainties. It is therefore important to examine the influence of

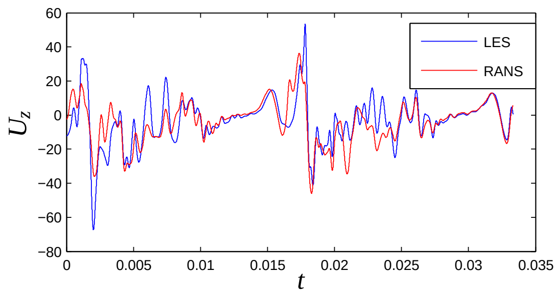

Figure 5. Fluctuations of U_z for 2 periods computed by RANS and LES, f=60 Hz

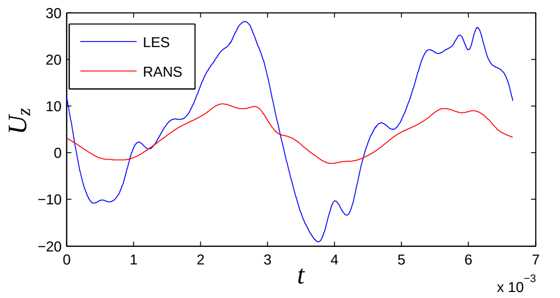

Figure 6. Fluctuations of U_z for 2 periods computed by RANS and LES, f=300Hz

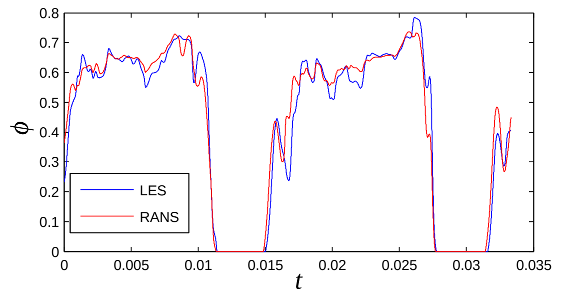

Figure 7. Scalar fluctuations inside the shear layer for 2 periods computed by RANS and LES for f=60 Hz

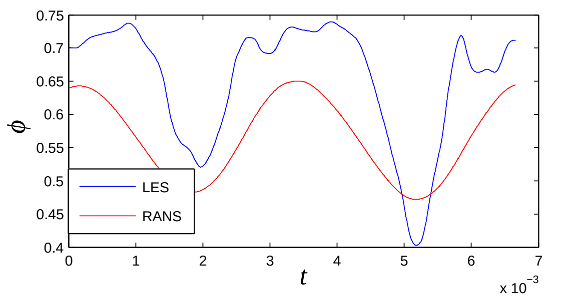

Figure 8. Scalar fluctuations inside the shear layer for 2 periods computed by RANS and LES, f=300Hz

the boundary conditions on the results.
In this study a stationary EGR flow will be compared to pulsating EGR flow, i.e. sine-shaped pulsations are defined on the EGR inlet with an amplitude of 50 % of the mean flow and a frequency of 3 times the rotational speed of the engine, i.e. each pulse corresponds to one cylinder valve opening (one engine cycle corresponds to two revolutions). The mean EGR concentration is set to 30%. At the outlet the mass flow to the cylinders is simply assumed as triangular functions during the opening time of the valves. The specified outlet mass flow is shown in Fig. 10. These cylinder valve timings correspond to 1200 rpm.

As can be seen in Fig. 9 the flow is highly unsteady even for stationary inlet conditions. A look on the flow field in a cut parallel to the main flow direction (see Fig. 11) reveals some of the flow mechanisms. Past the second bend, there is a recirculation zone where high shear and reverse flow are occurring. This causes high turbulence intensities which is promoting the mixing in this region. Fig. 12 shows the instantaneous concentration for constant EGR inflow. Due to the circulation induced by the double-bended pipe upstream of the EGR inlet, the EGR gases are moved along the pipe walls to the back side of the manifold.
In spite of the complexity of the geometry and the high turbulence levels, the mixture in the region of the cylinder inlets is far from being homogeneous. Both in the LES and the RANS computations, there are instantaneous differences of up to 10 % predicted. As in the T-junction case, the RANS computations imply less turbulent diffusivity for stationary EGR flow.
Fig. 13 gives the correspondent concentration for the pulsating EGR inflow. The pulses can clearly be seen travelling through the manifold. The pulses increase the concentration differences and are diffused only slowly. Also here, RANS and LES agree better than for the stationary case.
In engine applications, one is interested in the actual EGR rate of the flow into the cylinders. Fig. 14 shows a comparison of the EGR rate under the time of one valve opening of valve 1 for all used methods and boundary conditions. Both turbulence approaches predict high fluctuations and inhomogeneity.
In order to evaluate the inhomogeneity among the cylinders, the EGR flow into the cylinders is computed by integrating the EGR rate over the cylinder opening time. The results are given in table 2. In average the EGR concentration is quite homogeneous, the deviations are between $\pm 2\%$. 2% less EGR might however result in a drastic increase of NOx emissions, since they are very sensible to the EGR rate. Moreover the cycle-to-cycle variations have to be taken into account. These are in the order of 2-3% for the LES computations. The cycle-to-cycle variations can not be seen in the RANS computations. It can also be expected, that the cycle-to-cycle variations become less uniform at higher engine speeds, due to the fact that the opening times become shorter.

Conclusions

A systematic comparison of the computation of mixing processes in different geometries with RANS using the k-ε-model and LES has been performed. First, the flow in a T-junction with circular cross-section was considered for stationary and pulsating flow. For stationary flow the RANS method failed in predicting the correct scalar distribution. For pulsating inflow conditions with low frequencies, LES and

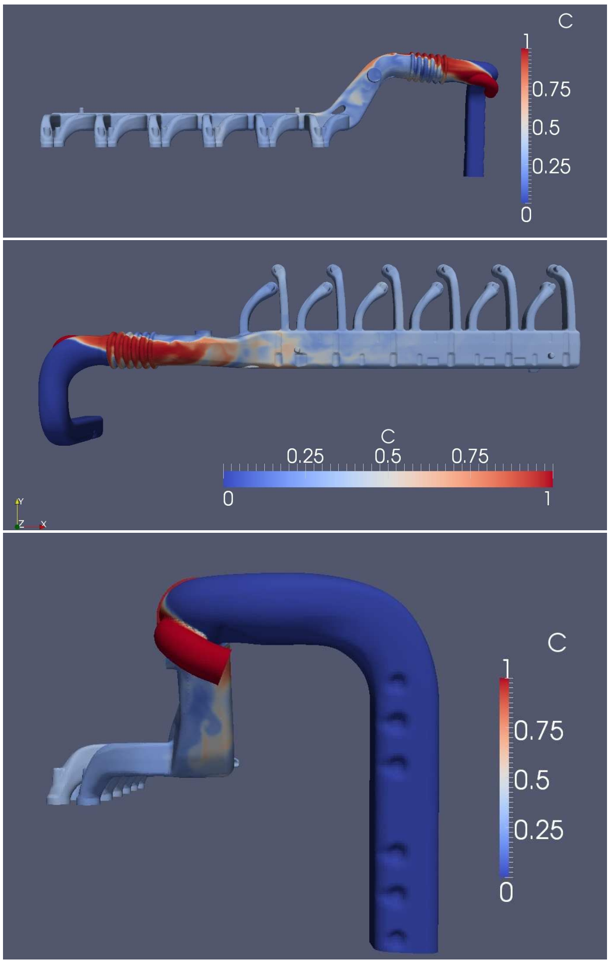

Figure 9. Inlet manifold provided by Scania including instantaneous concentration computed by LES with constant EGR flow

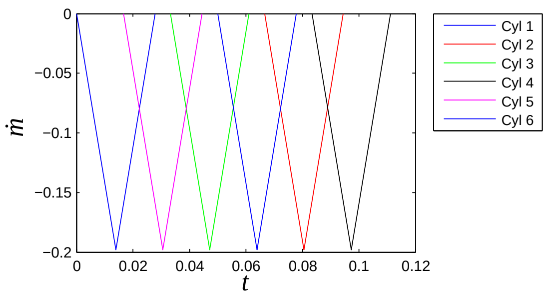

Figure 10. Time dependent mass flow specified on the outlet boundaries

RANS stat	32.2	30.3	29.7	29.5	29.7	30.7
LES stat	28.1	29.0	29.8	30.6	30.7	31.7
RANS puls	29.8	30.8	30.4	29.5	29.7	30.8
LES puls	31.9	31.7	30.6	29.2	29.8	30.3

Table 2. Mean of the EGR concentration into each of the (columns) cylinders in %, averaged over 4 engine-cycles

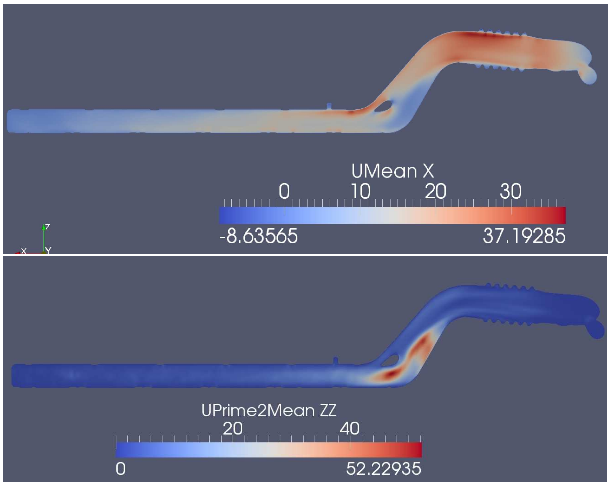

Figure 11. Mean velocity in x-direction (top) and $\overline{u_z' u_z'}$ (bottom) computed by LES with constant EGR flow

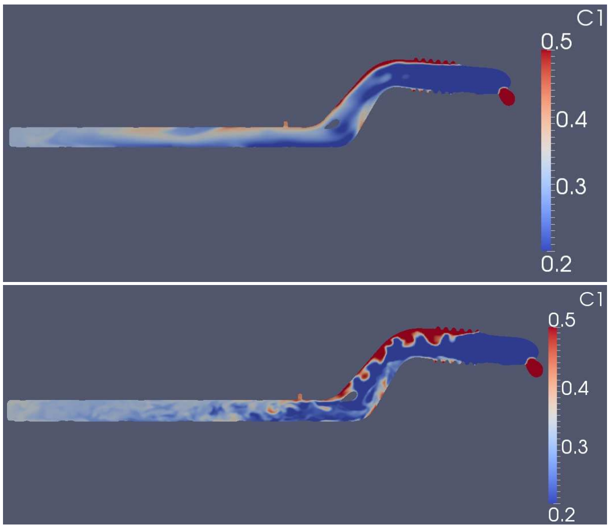

Figure 12. Instantaneous concentration for the same instant of time computed by RANS (top) and LES (bottom) for constant EGR flow

RANS agree fairly well, because the scalar is governed by the pulsations rather than the turbulence modeling. In the case of pulsation frequencies that are in the same order as the turbulent scales, an interaction occurs and the flow cannot be described as quasi-stationary. These effects cannot be predicted well by URANS.

The computation of the flow in a Scania Diesel engine manifold has shown that the flow is significantly inhomogeneous. Pulsations coming from the EGR side are travelling through the manifold and are mixed very slowly. The pulsations must therefore be taken into account, when computing EGR distributions. The major difference between RANS and LES in these computations is that the cycle-to-cycle variations cannot be captured by URANS.

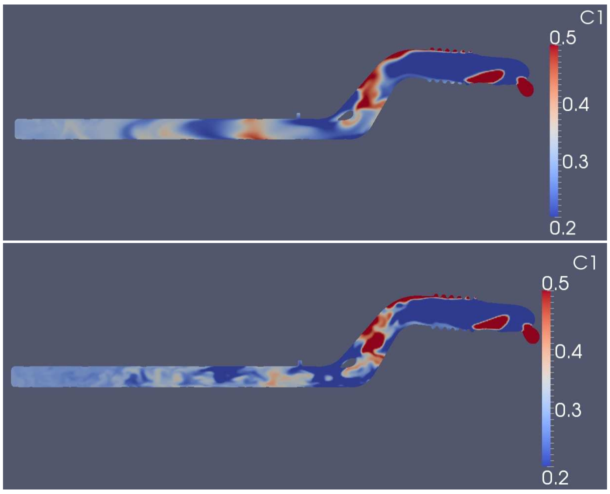

Figure 13. Instantaneous concentration for the same instant of time computed by RANS (top) and LES (bottom) for pulsating EGR flow

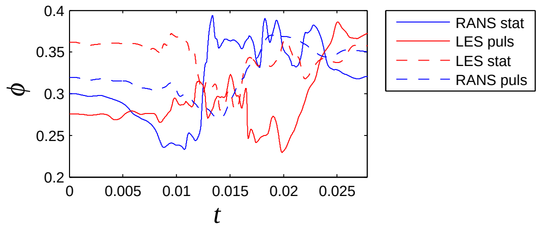

Figure 14. Sample of the EGR rate during one valve opening close to the cylinder port

Acknowledgements

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