LARGE EDDY SIMULATION OF A TURBULENT HYDROGEN DIFFUSION FLAME

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ABSTRACT

In this work a large eddy simulation (LES) of a turbulent hydrogen jet diffusion flame is presented. The numerical method handles fluctuations of density in space and in time, but assumes density to be independent of pressure (incompressibility). The chemical composition of the fluid is described by solving the transport equation for mixture fraction f. Density, viscosity, temperature and species mass-fractions are evaluated assuming chemical equilibrium. To account for sub-grid fluctuations of f, its sub-grid distribution is presumed to have the shape of a β-function.

The first part of the discussion addresses the influence of inlet boundary conditions and the range close to the nozzle. LES shows to be capable of providing an accurate description of this area. In the second part of the discussion, radial profiles at different axial positions are shown for a complete set of statistically evaluated quantities, i.e. mean velocity, Reynolds-stress tensor, means and variances of mixture fraction and temperature. The results of the LES calculation match experimental data very well. Though the methods applied are of moderate complexity and numerical cost, they prove to be adequate for the considered flow.

INTRODUCTION

Large-eddy simulation (LES) is a method of great potential for the simulation of turbulent diffusion flames, because fluctuations of velocity and chemical composition are resolved down to filter width. Hence, an accurate description of mixing, the driving mechanism of combustion in such systems, is possible. Though improvements are achieved continuously, many works imply major simplifications. When using elaborated chemistry models, often the Navier-Stokes equations are solved only in two dimensions in order to reduce the computational cost (Calhoon and Menon, 1996), (Colucci et al., 1998). Thus, the three-dimensional nature of turbulence is neglected. Sometimes only simple configurations of flow like isotropic turbulence are considered (Cook and Riley, 1994), (Menon et al., 1996). A very strong simplification for LES of reacting flows is to restrict density to be constant is space and time. It is applied even in recent works (Calhoon and Menon, 1996), (Colucci et al., 1998), (Cook and Riley, 1998), (deBruynKops et al., 1998). While such simplifications are acceptable for studying fundamental phenomena, they can not be applied to flow configurations occurring in technical applications.

In the current paper results from the simulation of a reacting flow using LES without the mentioned restrictions are presented. The chosen configuration is a turbulent hydrogen jet diffusion flame, for which a complete set of experimental data is available (EKT, 1997). The numerical method used for the simulation assumes density to independent of pressure, which is a reasonable approximation for the considered low Mach-number flow. Yet, spatial and temporal fluctuations of density are treated. This requires a time integration method different from the constant density case. For the current calculations, the pressure correction scheme used traditionally for LES of isodensity flows has been extended appropriately.

NUMERICAL PROCEDURE

The flow field of the jet flame is described by the filtered equation of continuity together with the three-dimensional filtered Navier-Stokes equations for variable density fluids.

$$\frac{\partial \bar{\rho}^{\Delta}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}^{\Delta}\tilde{u}_j^{\Delta}\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}^{\Delta}\tilde{u}_i^{\Delta}\right) = -\frac{\partial}{\partial x_j}\left(\bar{\rho}^{\Delta}\tilde{u}_i^{\Delta}\tilde{u}_j^{\Delta}\right) - \frac{\partial \bar{p}^{\Delta}}{\partial x_i} + \bar{\rho}^{\Delta} g_i + \frac{\partial}{\partial x_j}\left[\bar{\mu}^{\Delta}\left(\frac{\partial \tilde{u}_j^{\Delta}}{\partial x_i} + \frac{\partial \tilde{u}_i^{\Delta}}{\partial x_j}\right) - \frac{2}{3}\bar{\mu}^{\Delta}\frac{\partial \tilde{u}_k^{\Delta}}{\partial x_k}\delta_{ij} + \bar{\rho}^{\Delta}\tau_{ij}^{\mathrm{sgs}}\right] \tag{2}$$

Sub-grid scale stresses τ_{ij}^{sgs} are closed using Germano's (1991) dynamic procedure. In order to stabilize the model, the modification proposed by Lilly (1992) is applied and negative values for the parameter C of the underlying Smagorinsky-model are clipped. Because the Mach-number of the flow is low, density is assumed to be independent of pressure (incompressibility). The chemical composition of the flow is described by solving the filtered transport equation

$$\frac{\partial}{\partial t}\left(\bar{\rho}^{\Delta}\tilde{f}^{\Delta}\right) = -\frac{\partial}{\partial x_j}\left(\bar{\rho}^{\Delta}\tilde{f}^{\Delta}\tilde{u}_j^{\Delta}\right) + \frac{\partial}{\partial x_j}\left(\frac{\bar{\mu}_{\mathrm{eff.}}^{\Delta}}{\sigma_f}\frac{\partial \tilde{f}^{\Delta}}{\partial x_j}\right) \tag{3}$$

for mixture fraction f. Assuming chemical equilibrium, density, viscosity, temperature and species mass-fractions are evaluated as functions of Favre-filtered mixture fraction $\tilde{f}^{\Delta}$ and its sub-grid variance $\overline{f''^2}^{\Delta}$. The latter is approximated by the resolved fluctuations in a domain of twice the size of a grid cell. The shape of the sub-grid distribution of f is presumed on basis of the β-function.

Equations (1), (2) and (3) were transformed into cylindrical coordinates and discretised in space by finite volumes utilizing central schemes. The accuracy of approximation is 4th order for convective terms and 2nd order for all other terms. The equations are integrated in time by a 3rd order low-storage Runge-Kutta method, pressure is determined by solving a Poisson equation derived from the equation of continuity. Because density varies in time, $\frac{\partial \bar{\rho}^{\Delta}}{\partial t}$ appears as source term in this equation. Time integration of equation (3) yields the new value for $\overline{\rho f}^{\Delta}$, not for $\tilde{f}^{\Delta}$. Hence, in order to determine $\bar{\rho}^{\Delta}$, at every stage of the time integration and for each grid cell the non-linear equation

$$F(\tilde{f}^{\Delta}) = \bar{\rho}^{\Delta}\left(\tilde{f}^{\Delta}, \overline{f''^2}^{\Delta}\right) \cdot \tilde{f}^{\Delta} = \overline{\rho f}^{\Delta} \tag{4}$$

has to be solved. Figure 1 shows, that depending on the values of $\overline{f''^2}^{\Delta}$ and $\overline{\rho f}^{\Delta}$ there may be several solutions to (4). The procedure described in (Forkel and Janicka, 1999) is used to determine all solutions efficiently. The one closest to the old value of $\tilde{f}^{\Delta}$ is chosen to be the new one. By the assumption of incompressibility, acoustic modes have been removed from all quantities, but high-frequency errors occur due to low-diffusive spatial discretisation. To stabilize the method, these are removed from density by relaxing it in time. For the present calculations the relaxation time was set to be $t_{\mathrm{relax}} = 5 \cdot 10^{-4}$ seconds.

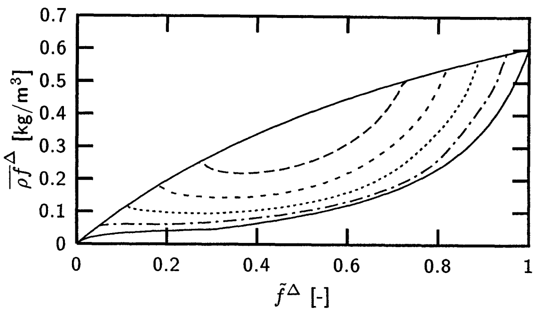

Figure 1: $\overline{\rho f}^{\Delta}$ as a function of $\tilde{f}^{\Delta}$ and $\overline{f''^2}^{\Delta}$. Lines bottom to top: $\overline{f''^2}^{\Delta} = 0, 0.05, 0.1, 0.15, 0.2, 0.25$ (fuel: H_2/N_2, 50% vol. each, ox.: air)

CONFIGURATION OF FLOW

The considered flow is test case "H3" defined for the Second International Workshop on Measurement and Computation of Turbulent Non-Premixed Flames (Barlow, 1999).

Experimental Setup

It is a turbulent jet diffusion flame combusting a mixture of H_2 and N_2, 50% vol. each. The fuel discharges from a circular nozzle of diameter 8 mm at bulk velocity 34.8 m/s into air co-flowing at 0.2 m/s. The corresponding Reynolds-number is 10,000, Froude-number is 15,500. A full data set for this configuration is available from experiments using LASER-Doppler-velocimetry (velocity components, turbulence quantities) and combined Raman-/LIF-spectroscopy (chemical composition, temperature). All data and a more detailed description of the experimental setup are accessible on the WWW (EKT, 1997).

Computational Domain, Boundary Conditions

The LES have been carried out on a cylindrical computational domain of 48 nozzle diameters D length and Radius $30D$. The numerical grid consisted of $257 \times 32 \times 60$ cells (axial $\times$ circumferential $\times$ radial). Radial grid spacing was 5 equidistant cells over the radius of the nozzle and stretching on the outside with a constant ratio of 1.05 between two cells. The grid was equidistant in the other two directions.

Two different methods were applied to generate inflow boundary conditions at the location of the nozzle. For the calculation labelled 'LES coupled' in the figures below, a LES of fully developed pipe flow was carried out in parallel. The instantaneous velocity profile at a fixed axial position in the pipe was posed in the exit plane of the nozzle. The calculation labelled 'LES random' uses random forcing instead with profiles for mean and variances of the velocity components iden-

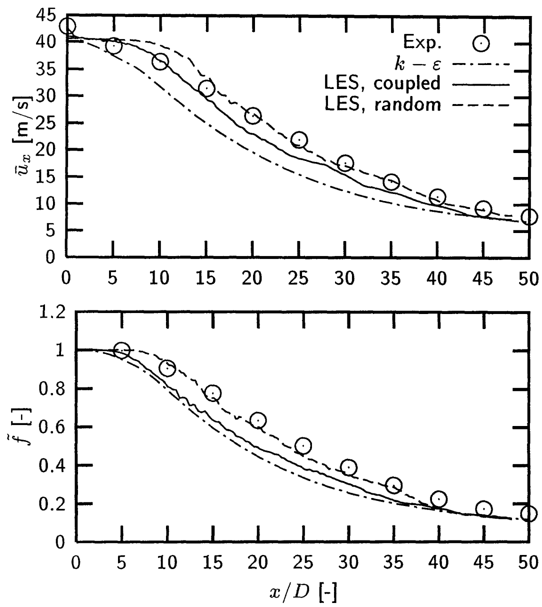

Figure 2: Centerline decay of velocity (Reynolds-mean) and mixture fraction (Favre-mean). $k-\varepsilon$ simulation: both quantities Favre-averaged

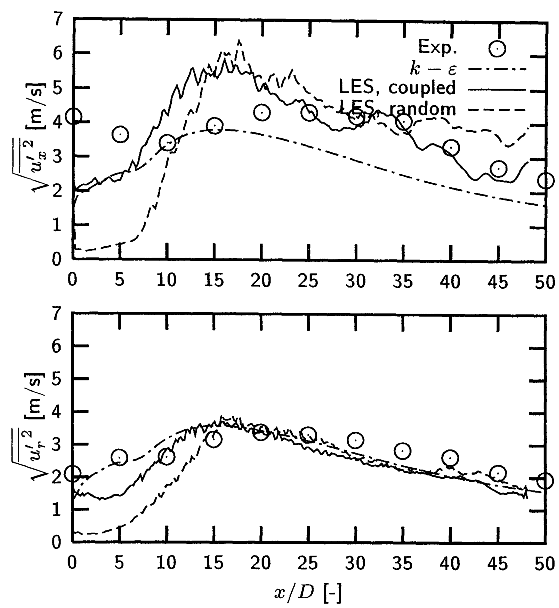

Figure 3: Fluctuations of axial and radial velocity components on the centerline ($k-\varepsilon$: Favre-based, others: Reynolds-based)

tical to case '**LES coupled**'. On the downstream axial boundary zero gradient conditions are posed with negative axial velocities being clipped. Hence, temporary inflow is prohibited. On the outer radius of the computational domain fixed absolute values for pressure are prescribed. The velocity component normal to this boundary is determined by solving a modified momentum equation in order to allow for entrainment. Zero gradients are posed for the other two components. Periodicity is applied for all quantities in the circumferential direction.

DISCUSSION OF RESULTS

The LES calculations are compared to experimental data and to results obtained from a Reynolds-averaged Navier-Stokes (RANS) simulation using the $k-\varepsilon$ model. Because measured data was available only for statistical moments (means, variances, correlations), the discussion is restricted to these quantities. LES allows for the calculation of both Reynolds- and Favre-means. In the figures below always the same averaging is shown as for the experimental data. Please notice, that the RANS simulation provides only the Favre-means.

Influence of Inlet Boundary Conditions

Figure 2 shows the centerline decay of mean axial velocity $\bar{u}_x$ and mixture fraction $\tilde{f}$. LES with inlet profiles generated by pipe flow simulation (**LES coupled**) gives a good approximation of velocity close to the nozzle, but further downstream $\bar{u}_x$ is a bit too low. The shape of the mixture fraction profile corresponds well to the experiment, but its decay begins too early. As a consequence, the calculated values are too low. When using random forcing in the nozzle (**LES random**) instead of coupling to pipe flow, the decay of velocity and mixture fraction is shifted downstream by approximately 5 nozzle diameters D. The axial profiles for both mean quantities match the measured data very well.

The reason why changing the inlet boundary condition has this effect can be seen by looking at the axial profiles of velocity fluctuations (figure 3). Though the root mean square (rms) on the boundary is identical for both LES, it drops immediately to a fraction of the forcing level when random forcing is applied. This has the consequence, that velocity fluctuations in the shear layer close to the nozzle are too small (figure 4, bottom) which in turn delays the breakup of the jet. Inlet profiles generated by a pipe flow simulation on the other hand provide fluctuations correlated according to the physics of the flow. Hence, the velocity fluctuations in the shear layer can be simulated much better. These results confirm the observation made by Weinberger et al. (1997) in the case of an isothermal jet, that it is necessary to provide the proper turbulent structures on the boundary in order to get a good prediction of the flow close to the nozzle.

However, in the experimental setup the velocity field in the exit plane of the nozzle does not correspond to fully developed pipe flow. Figure 3 (top) shows that the measured rms of u_x at $x/D = 0$ on the axis is twice as large as the value of the pipe flow boundary condition of '**LES coupled**'. Further investigations are

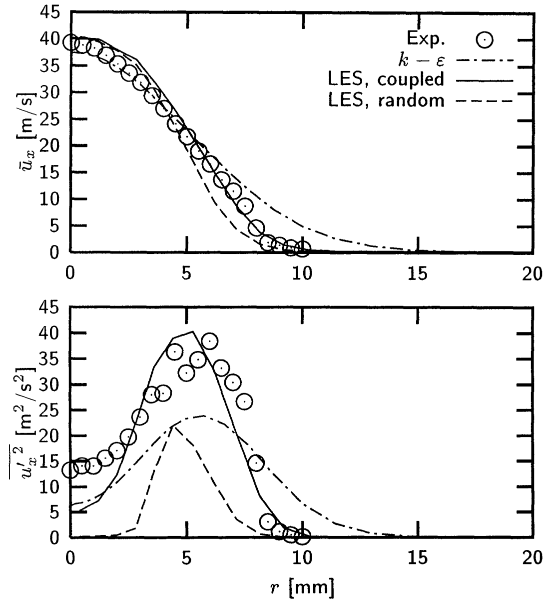

Figure 4: Radial velocity profiles at $x/D = 5$. Reynolds-mean and variance of axial component ($k - \varepsilon$: Favre-mean)

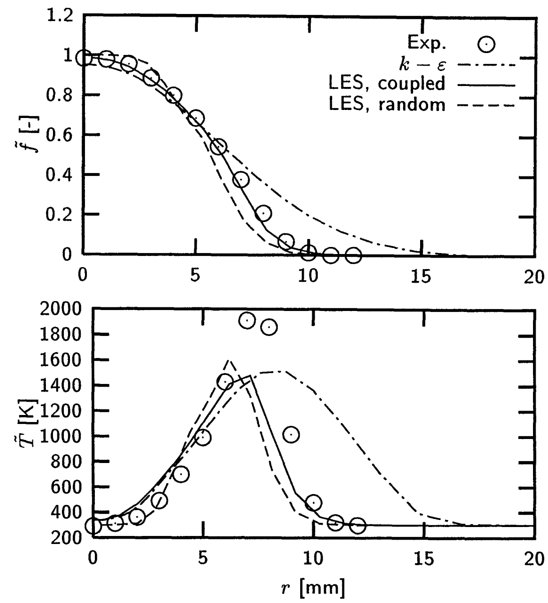

Figure 5: Radial profiles of mixture fraction and temperature at $x/D = 5$. (Favre-means)

necessary in order to develop inlet boundary conditions that correspond to given profiles for mean velocity and fluctuations while providing proper spatial correlations. Fortunately, the influence of inlet boundary conditions on the downstream region is small. For $x/D > 15$ both LES show almost the same rms-values on the axis. Also, the influence on the width of the jet flame is small, there is only a small change in radial profiles for mean axial velocity (figure 4, top) and scalars (figure 5).

For reference, figures 2 through 5 include results from a RANS simulation using the $k - \varepsilon$ model. The profiles of mean velocity and mixture fraction decay too quick on the centerline (figure 2). In the experiment and in both LES $\tilde{f}$ remains constant until $x/D = 5$, but it begins to decay immediately in the $k - \varepsilon$ simulation. The calculated spreading of the jet flame is too wide. Errors become smaller with increasing axial distance from the nozzle, which indicates that the $k - \varepsilon$ model is suitable for the simulation of the downstream region, but compared to LES it performs poorly. This can be explained by the fact, that LES allows a very detailed representation of the turbulent structure of the flow both on the boundary and in the shear layer. In contrast, for RANS all this information is reduced to very few parameters.

Radial Profiles

Figures 6 and 7 show radial profiles at axial positions $x/D = 20$ and $x/D = 40$ for the LES using the random forcing inlet condition. Radial profiles from the LES coupled to pipe flow (not shown) are very similar, except for the fact discussed in the last section, that mean values on the axis are lower by a small amount.

At both axial positions mean velocity profiles agree very well to the measured data, but variances of the axial component are too high near the axis. This may be caused by the use of a cylindrical grid for the discretisation, which results in a reduced order of approximation on the axis. All other non-vanishing components of the Reynolds-stress tensor are simulated well. Mean and fluctuations of mixture fraction correspond well to the experiment at axial position $x/D = 20$, at $x/D = 40$ the mean is too low on the axis. Temperature is a function of mixture fraction in the simulation, means are predicted well at both axial distances, but fluctuations are somewhat too high. Again, errors are larger close to the axis. Despite the described differences, the general agreement of values calculated using large eddy simulation and measured data is very good.

SUMMARY AND CONCLUSIONS

Large eddy simulations of a turbulent hydrogen jet diffusion flame utilizing two different inlet boundary conditions have been carried out. There were difficulties in getting both a good description of turbulent fluctuations close to the nozzle and an accurate prediction of the position where the axial decay of mean velocity and mixture fraction begins. However, the results obtained from both LES agree much better with measurements than those from a $k - \varepsilon$ simulation. Radial profiles at different axial positions show, that LES is capable of a very accurate simulation of the presented flow.

Though the computational cost of the LES has been higher than for RANS due to fully three-dimensional

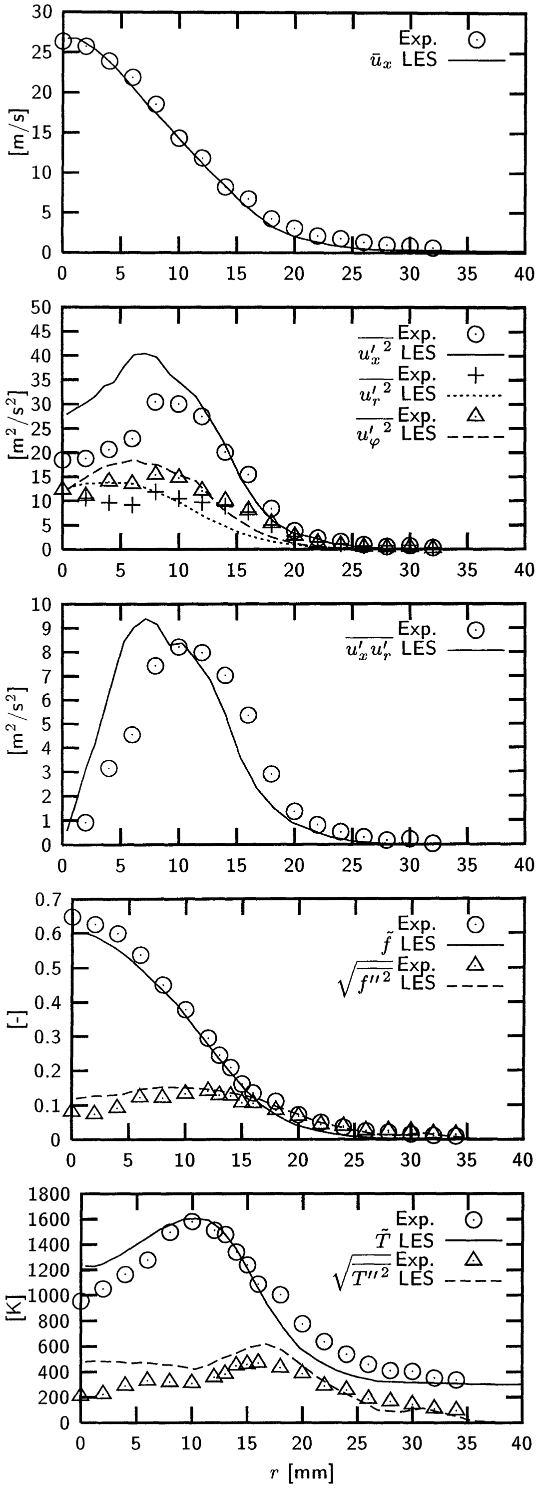

Figure 6: Radial profiles at $x/D = 20$

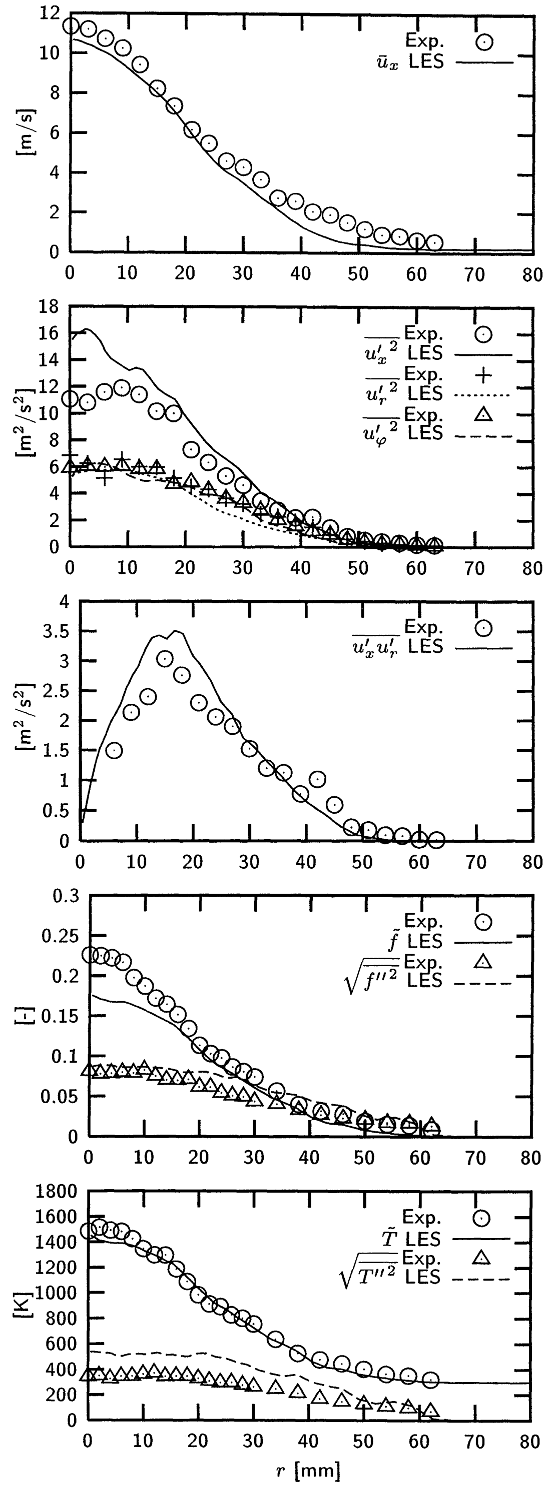

Figure 7: Radial profiles at $x/D = 40$

instationary solving of the Navier-Stokes equations, it was still possible to perform all calculations on a workstation.

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