MIXING IN ISOTROPIC TURBULENCE WITH SCALAR INJECTION AND APPLICATIONS TO SUBGRID MODELING

Marc Elmo[1], Jean Pierre Bertoglio[1] and Vladimir A. Sabel'nikov[2]

[1]Laboratoire de Mecanique des Fluides et d'Acoustique UMR 5509
Ecole Centrale de Lyon
36 Av. Guy de Collongue, 69130 Ecully, FRANCE

[2]TSAGI, Zhukovsky
Moscow Region 140160, RUSSIA

ABSTRACT

A new technique for injecting scalar fluctuations in a DNS of isotropic turbulence is presented. It is used to study statistically steady states associated with different levels of mixing. The results are analysed in terms of p.d.f and they are used as a data base to investigate the effect of the filtering operation that is performed in the case of a LES. It is shown that the p.d.f of the scalar is substantially affected by the filtering operation. It is also shown that the Cook and Riley (1994) subgrid model allows to reconstruct a p.d.f which is in fairly good agreement with the unfiltered DNS results.

INTRODUCTION

The mixing of a passive scalar by turbulence is of interest for many practical applications. For problems such as combustion, a description of the scalar field by low order statistical moments is insufficient to account for the non linear nature of the chemical reaction term. Indeed what is needed is an estimation of the probability density function (p.d.f) of the scalar fluctuation. It is well known that the equation governing the evolution of the p.d.f is not closed. It contains terms like the conditional scalar dissipation which are unknown and need to be modeled. For turbulent reactive flows it is also important to understand and predict situations in which the mixing is not complete. Another issue is the influence of the length scale at which the scalar fluctuations are created or injected in the flow. These considerations have led us to investigate the behaviour of the p.d.f of the scalar fluctuation in a simple case of homogeneous isotropic turbulence in which the scalar is injected by a new forcing technique in a Direct Numerical Simulation (DNS). This technique allows to control the scalar length scale as well as to investigate situations corresponding to different levels of mixing and is presented in the next section.

For real flow computations at high Reynolds number encountered in the description of practical problems, Large Eddy Simulation (LES) appears to be the most reasonable way to predict the mixing with a good accuracy. In particular, capturing the dynamics of the large eddies is an important feature for predicting the mixing since the large scales are initiating the transfer of scalar fluctuations to the small scales. This kind of simulation involves a filtering operation removing the scalar fluctuations at small scales, and requires the introduction of a subgrid model to account for the effect of the small eddies and of the scalar dissipation. The filtering operation was shown to affect the shape of the scalar p.d.f by Jiménez et al. (1997) who also have shown, using *a priori* tests in the case of a mixing layer, that improved subgrid models (Cook and Riley 1994) can satisfactorily take into account the contribution from the small scales to the scalar statistics. In the present paper the same problem is addressed in the case of isotropic turbulence with scalar injection. A top hat filter is therefore introduced in our DNS results to investigate the effect of the filtering on the scalar. A Large Eddy Simulation of the same flow is also performed in order to make an *a posteriori* study of the ability of an eddy diffusivity to model the effect of the small scales on the mixing.

NUMERICAL METHOD AND INJECTION TECHNIQUE

The incompressible Navier Stokes equation and the convection diffusion equation for the scalar c are integrated using a pseudo-spectral method. These equations are solved in a three dimensional cubic domain of size L, with periodic boundary conditions on both the velocity and scalar. The time stepping scheme is a second-order Runge Kutta method. The DNS are performed at a resolution of 128^3 grid points. A random forcing is applied in the low wave-number range of the velocity spectrum. It can be alternatively white-noise or time correlated (generated using a Langevin equation). This forcing leads to obtain a statistically steady homogeneous and isotropic velocity field.

The scalar forcing technique consists in refreshing the field by operating an injection of fluctuations in physical space. This operation is repeated periodically in time, with a period T_i. The basic outline of the forcing can be described as follows. In the computational domain (of size L), n subboxes of size l are randomly selected. In one half of these subboxes (n/2), $c(x) = +1$ is imposed, whereas $c(x) = -1$ is imposed on the other half. This procedure essentially leads to a forcing function whose p.d.f is bi-modal. The choice of l/L allows to keep control upon the scalar integral length scale L_c and correlatively on the ratio $R_l = \frac{L_c}{L_u}$ where L_u is the velocity integral length scale. L_u and L_c are defined by:

$$L_u = \frac{3\pi}{4} \frac{\int_0^\infty \frac{E_u(k)}{k} dk}{\int_0^\infty E_u(k) dk}$$

$$L_c = \frac{\pi}{2} \frac{\int_0^\infty \frac{E_c(k)}{k} dk}{\int_0^\infty E_c(k) dk}$$

where $E_u(k)$ and $E_c(k)$ are respectively the velocity and scalar spectra. A characteristic time of injection is

$$T_{res} = T_i * (\frac{L^3}{n v_f})$$

where v_f is the volume of a forced subbox. The choice of the time scale ratio

$$R_t = T_{res}/T_{turb}$$

where $T_{turb} = \frac{L_u}{u'}$ (u' being the r.m.s value of the fluctuation velocity) is the eddy turnover time of the turbulent field, governs the level of mixing.

DNS RESULTS

The simulations are performed at a Reynolds number (based on the integral length scale) equal to 90 and a Schmidt number equal to 1. For all the results presented in the paper, the integral length scale ratio R_l is set equal to 0.71. Fig.1 shows the time evolution of the scalar r.m.s value ($\sigma = \sqrt{< c^2 >}$) for two time scale ratios, $R_t = 0.35$ and $R_t = 2.2$. It is seen that a statistically steady state is reached. Results are then averaged over the stationary state. In Fig.2, where the spectrum of the scalar fluctuation is plotted for $R_t = 2.2$, it can be observed that, although the Reynolds number is quite low, a $K^{\frac{-5}{3}}$ range seems to be detected in the scalar spectrum. Fig.3 shows the p.d.f of the scalar for three time scale ratios, $R_t = 0.35$, $R_t = 1.1$ and $R_t = 2.2$. For $R_t = 0.35$ two peaks are clearly observed close to ± 1 indicating a high level of unmixing. The peaks are much smaller when $R_t = 2.2$ and, for small and moderate amplitude fluctuations, the p.d.f has a shape characteristic of a better mixed situation. The p.d.f for $R_t = 1.1$ is also given as an example of an intermediate situation. Analysis of the conditional dissipation (not presented here) leads to conclude that, for the unmixed situations, the high values of the p.d.f at ± 1 correspond to unmixed blobs associated with a low dissipation rate.

APPLICATION TO L.E.S. AND SUBGRID P.D.F MODELING

In the case of a LES only the large scales of the field are computed. The key problem for applications of LES to reacting flows is therefore whether the subgrid models used to account for the small scales can properly reproduce the statistics of the whole field.

The problem is indeed twofold, the first question being whether the effect of the unresolvable scales on the dynamics of large scales of the concentration and velocity fields can be correctly taken into account (by eddy diffusivity and eddy viscosity types of subgrid models for example). The second question is whether the contribution of the small scales to the scalar statistics (and in particlular to the p.d.f which is needed to evaluate the reaction term) can be satisfactorily modeled.

In the present paper the second question is essentially addressed and use is made of the DNS results presented in the previous section to perform an *a priori* test of the Cook and Riley (1994) subgrid model.
The filtering operation for this test is performed in physical space by a top hat filter of width h:

$$\bar{c}(\vec{x}, t) = \frac{1}{h^3} \int\int\int_V c(\vec{x'}, t) d\vec{x'} \quad (1)$$

where c is the scalar fluctuation, $\bar{c}$ the filtered fluctuation and V the volume of the cubic domain of width h centered on $\vec{x}$.

We now intend to reconstruct the complete scalar p.d.f by modeling the scalar distribution at small scales. The β-assumed p.d.f approximation allows to generate a family of p.d.f (bounded at extremal values) associated with very different levels of mixing. It is often used to evaluate the distribution of the full scalar in practical problems (Miller et al. (1993)). Following Cook and Riley (1994) the β distribution is used here to approximate the scalar p.d.f at small scales. This technique was also used by Jimenez et al. (1997) and Réveillon and Vervisch (1996). The β distribution has the form:

$$P_h(c) = \frac{(\frac{1+c}{2})^{a-1}(\frac{1-c}{2})^{b-1}}{B(a,b)} \quad (2)$$

in which a and b can be expressed in terms of the filtered scalar $\overline{c}$ and of the subgrid variance $\overline{c_s^2}$.
$a = (\frac{1+\overline{c}}{2})(\frac{(1+\overline{c})(1-\overline{c})}{\overline{c_s^2}} - 1)$ and $b = \frac{1-\overline{c}}{1+\overline{c}}a$

$$\overline{c_s^2} = \overline{c^2} - \overline{c}^2 \quad (3)$$

An estimation of the complete scalar p.d.f can then be obtained by the relation:

$$P(c) = \int P_c(\overline{c}, c_s) P_h(c, \overline{c}, c_s) d\overline{c} dc_s \quad (4)$$

where P_c is the joint p.d.f of the filtered scalar and the subgrid r.m.s value.

For a real LES computation , $\overline{c_s^2}$ needs to be estimated (which can be done by similarity arguments-see Cook and Riley (1994)). In the present paper $\overline{c_s^2}$ was directly deduced from the DNS using (3).

FILTERED RESULTS AND RECONSTRUCTED SCALAR P.D.F

To investigate the effect of the filtering operation in a Large Eddy Simulation the filter defined by (1) was applied to the DNS results. Two filter widths h1 et h2 ($\frac{h_1}{L} = \frac{1}{32}$, $\frac{h_2}{L} = \frac{1}{16}$) were used. The scalar p.d.f for the filtered and unfiltered results are compared in Figs.4-5 and 6, for three time scale ratios. It can be observed that the p.d.f of the filtered scalar exhibits smaller peaks at $c = \pm 1$, and a higher amplitude for small fluctuations, than the p.d.f of the unfiltered field. It can also be observed that the influence of the filtering is more important for the larger filter width. These results are in agreement with those of Jimenez *et* al. (1997). It has to be mentioned that the DNS results were slightly corrected before applying the filter: fluctuations larger than 1 (or smaller than -1) were assigned to be equal to 1 (or -1). This correction was introduced in order to avoid working with values of $\overline{c}$ outside the [-1:1] domain in the study presented below.

The filtered scalar is now used to test the reconstruction technique proposed by Cook and Riley (1994) and described above. The test is performed for the three cases of mixing and for the two filter widths. The reconstructed p.d.f are compared with the complete p.d.f in Fig.7-8-9 for $R_t = 2.2$, $R_t = 1.1$ and $R_t = 0.35$ respectively. It is seen that there is a good agreement between the reconstructed and the complete p.d.f. However, the reconstruction is less accurate when there is a high level of unmixing. It is also observed that, as could be expected, the p.d.f is reconstructed with more accuracy for the smaller filter width.

The above results were obtained using (3) to estimate the subgrid variance locally in the computational domain. In order to check the inportance of a local estimation, we also performed a test with an averaged estimation of $\overline{c_s^2}$ ($< \overline{c_s^2} >$, where $<>$ denotes the average over the numerical box). In figure 10 it is seen that the agreement with the DNS is less satisfactory for the averaged estimation of $\overline{c_s^2}$ than with the local one. This is particularly true for the large fluctuations where the averaged estimation leads to a strong overprediction of the p.d.f.

Another source of error in the case of a LES is the effect of the subgrid model on the resolved scalar field itself. This effect is investigated by *a posteriori* testing, that is to say by comparing the results of a real LES with the results of a filtered DNS. LES have been performed at resolutions of 32^3, 64^3 and 128^3 grid points with a spectral cut-off filter (at K_c), and with a spectral subgrid model (Chollet and Lesieur (1981)). The subgrid Schmidt number is equal to 0.7. In Fig.11 the scalar spectrum obtained with three different cut-off wave-numbers ($K_c = 2.8$, $K_c = 6$ and $K_c = 12.2$) are presented. It is seen that the $K^{-\frac{5}{3}}$ range detected in the case of DNS is confirmed by the LES. It is also seen that the shape of the spectrum is found not to depend on the cut-off wave number. In Fig.12 the p.d.f of the scalar obtained with LES when $K_c = 2.8$ is compared to the filtered DNS results. It is observed that the error remains small and that the overall shape of the p.d.f is well reproduced. However, when compared to the error associated with the subgrid scalar fluctuation (corrected using the Cook and Riley model (1994)) (Fig.7), the present error appears to be larger. Further comparisons, using different subgrid models, appear necessary before a definite conclusion could be reached. The Reynolds number effect should also be investigated, since in the present case we are comparing low Reynolds number DNS results with infinite Reynolds number LES.

CONCLUSION

DNS of isotropic turbulence were performed with an injection technique for scalar fluctuations leading to obtain statistically steady states associated with different levels of mixing characterized by different p.d.f shapes. It was shown that in the case of a LES the error induced by the filtering operation removing the small scale scalar fluctuations can be corrected by using the Cook and Riley subgrid model. Such a conclusion is in agreement with what was found by Jimenez *et* al. in the case of a temporally growing mixing layer.

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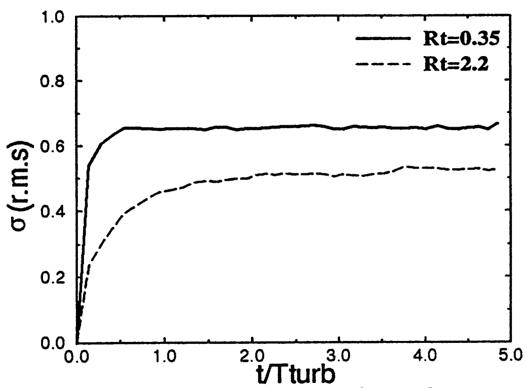

Figure 1: Time evolution of the scalar r.m.s value for two time scale ratios, $R_t = 0.35$ and $R_t = 2.2$ ($R_l = 0.71$).

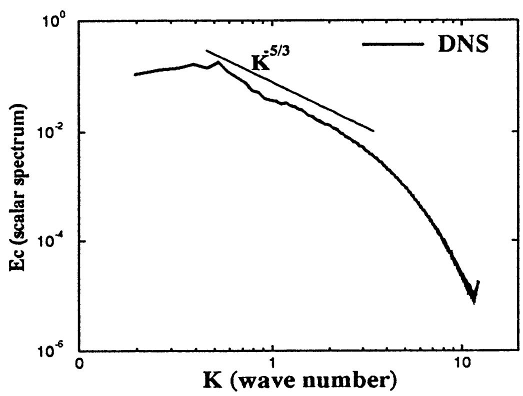

Figure 2: Scalar spectrum ($R_t = 2.2$).

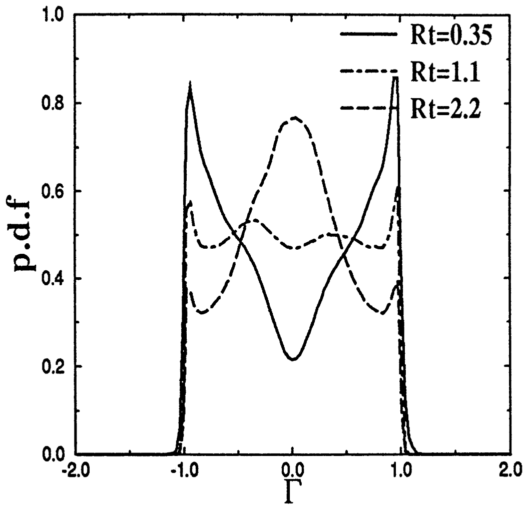

Fig.3 Probability density function of the scalar for three time scale ratios $R_t = 0.35$, $R_t = 1.1$ and $R_t = 2.2$ ($R_l = 0.71$).

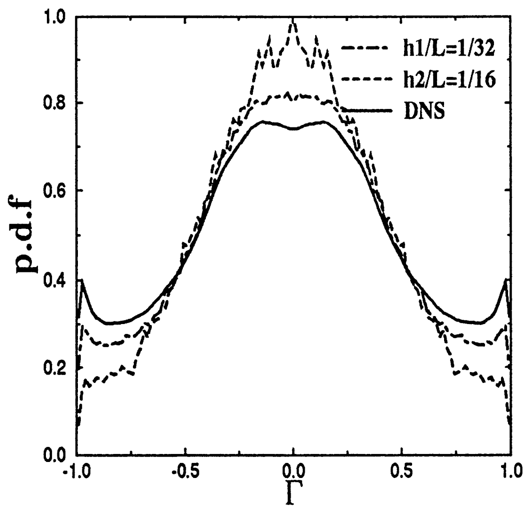

Figure 4: Probability density function of the scalar for filtered ($\frac{h_1}{L} = \frac{1}{32}$ and $\frac{h_2}{L} = \frac{1}{16}$) and unfiltered DNS results; $R_t = 2.2$, $R_l = 0.71$.

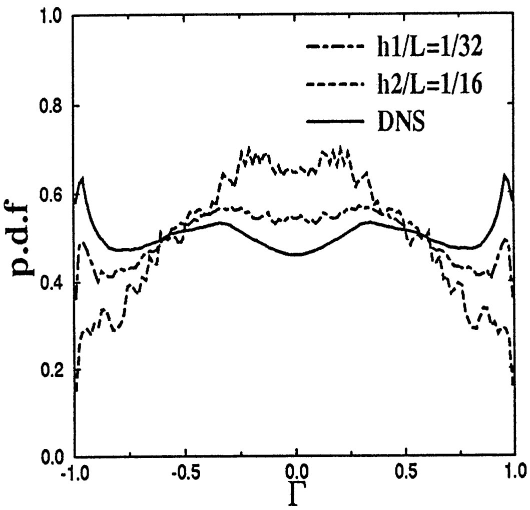

Figure 5: Same as Fig.4, but with $R_t = 1.1$.

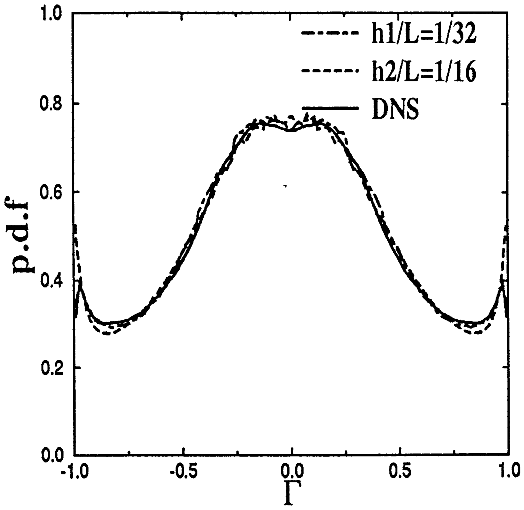

Figure 7: Reconstructed and true probability density function; $R_t = 2.2$.

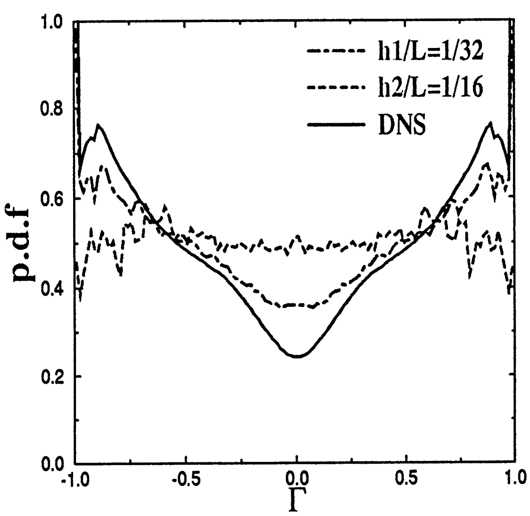

Figure 6: Same as Fig.4, but with $R_t = 0.35$.

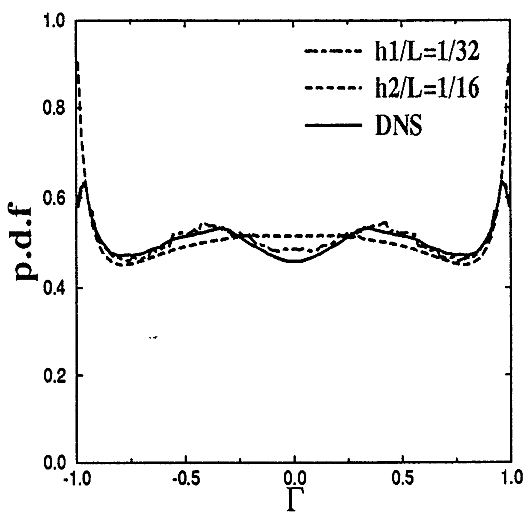

Figure 8: Same as Fig.7, but with $R_t = 1.1$.

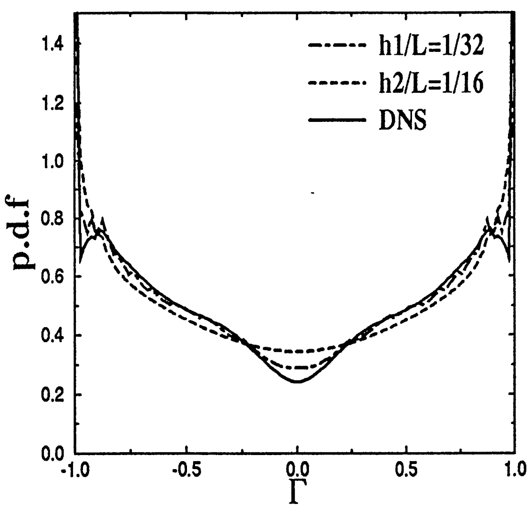

Figure 9: Same as Fig.7, but with $R_t = 0.35$.

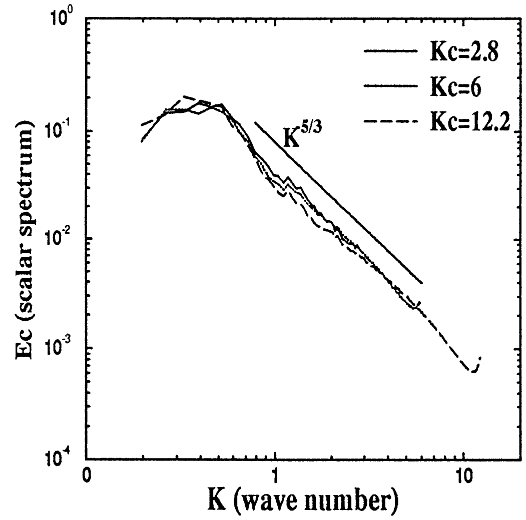

Figure 11: Scalar spectra for the LES with different cut-off wave-numbers $K_c = 2.8$, $K_c = 6$ and $K_c = 12.2$ ($R_t = 2.2$).

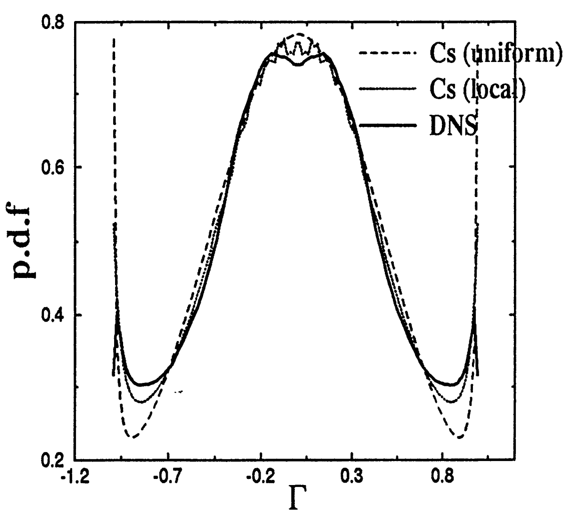

Figure 10: Reconstructed probability density function. Comparison between results obtained with local and averaged $\overline{c_s^2}$ ($h_2 = 2cm, R_t = 2.2$).

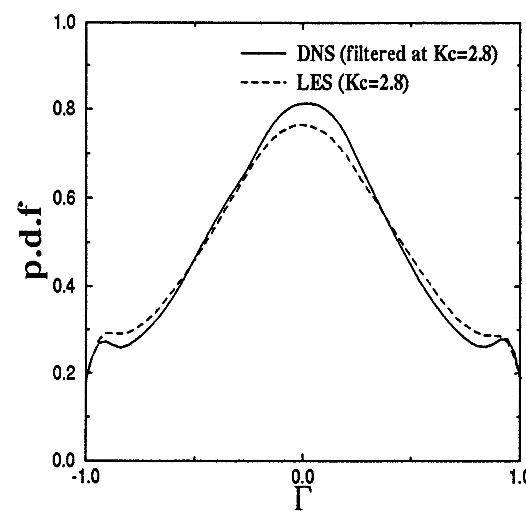

Figure 12: Comparison between the p.d.f of the filtered scalar (DNS) and the p.d.f of the scalar obtained by LES ($R_t = 2.2$).