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Development of a fractal-based LES model in PHOENICS

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ABSTRACT

This study concerns the development and validation of a new turbulence model for CFD simulations. The fractal theory of Mandlebrot (1974) and the dissipation-in-a-box formulation of Sreenivasan(1984) are used to determine local dissipation rates for use in a Large-Eddy-Simulation (LES) framework. Such a model has theoretical advantages over "industry-standard" two-equation models such as the k-ϵ, (a)because it removes some of the ambiguities associated with the formulation of the ϵ - turbulence energy dissipation equation and (b)it does not assume isotropy above the sub-grid dimension. The model is in fact simpler and numerically more stable than Reynolds stress closures and therefore more useful for engineering computations. The LES model of Ciofallo (1988) is attached to PHOENICS together with the fractal subgrid formulation given here, to create the FLES model.

1. INTRODUCTION

The behaviour of shear layers, laminar-turbulent intermittency regions, flame fronts and generally the interface between regions of high and low vorticity in a fluid display fractal characteristics. Mandelrodt (1974) was the first to relate fractals to the geometry of turbulence. The often observed spirals, rills, and turns in the fluid are fractals with planar dimensions, measured to be close to D=2.36 (Meneveau et al. (1987)). This dimensional consistency which was found to hold for a range of flows, including laboratory jets and wakes, grid turbulence and even large-scale atmospheric flows. It has been suggested that this unique dimension which is equivalent to that obtained in a 0.3/0.7 Cantor set, is due to the split of energy between eddies of various sizes in Kolmogorov's turbulent energy cascade. Recent research (Sakai et al. (1994)) has shown that there are deviations from this value. A constant dimension will be used in the development of our model.

Dissipation is the most uncertain quantity in any turbulence model. It is highly intermittent and it cannot be described well statistically, although researchers of the calibre of Kolmogorov (1962) attempted to do so (the so-called log-normal model). Dissipation is concentrated in areas of high vorticity, characterising the fractal interfaces. Dissipation, as shown by Frisch et al.(1985), is then a scalar fractal distribution, on a fractal base. To examine it, one may use multi-fractal mathematics.

Since fractals have the property of self-similarity at all scales, the classical eddy

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dissipation cascade in a box of a given size, may be described with an equivalent fractal cascade. In the context of CFD, the box is then a computational control volume (CV), and the integral quantity derived, is the total dissipation, ϵ within it. This idea may be used to develop a transport equation for ϵ, but then questions need to be answered regarding the anisotropy of turbulence (due to curvature or body force), and its effect on the base fractal dimension. More research is needed to provide the answers. Alternatively, we may assume that provided the "box" is very small, (a)transport is not very important, and (b)the eddies remain isotropic at small scales. A Large-Eddy-Simulation (LES) model may then be appropriate, in which case, anisotropy can be resolved, and the multi-fractal represents the subgrid dissipation ϵ_s from which a subgrid viscosity ν_s may be derived. These ideas form the foundation of the **FLES** model, as it has been named, which was first presented (in 2D), by the authors in Dempsey et al. (1994). The LES vehicle adopted to test this model, is the one presented by Ciofallo (1989); this is a spacial filtering model, as opposed to the spectral approach pioneered by Lesieur (1987).

This paper provides further details of the mathematical formulation and algorithmic development of the FLES method in a Control-Volume (CV) framework, and its application to two test-cases, a rectangular duct with wall heat transfer (2D) and gravity effects, and a backward-facing step (in 3D).

2. MATHEMATICAL FOUNDATION

2.1 Standard subgrid models

A full description of LES models is given, amongst others, in Voke and Collins(1983), Ferziger (1977), Moin and Kim (1982). The complete set of equations is (see Ciofalo(1988)),

$$\begin{aligned}
&\frac{\partial u_i}{\partial x_i} = 0 \\
&\frac{\partial u_i}{\partial t} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} - \frac{\partial u_i u_j}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\nu+\nu_s)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] \\
&\frac{\partial H}{\partial t} = -\frac{\partial u_j H}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\alpha+\alpha_s)\frac{\partial H}{\partial x_j}\right] \qquad (1) \\
&P = p + \frac{2}{3}\rho k_s
\end{aligned}$$

where, υ_s is the eddy viscosity, α_s is the thermal diffusivity and $\mathbf{k}_s$ is the turbulent kinetic energy (the subscript **s** denotes subgrid quantities). If υ_s is determined by the grid scale and ϵ_s is the total subgrid dissipation, then dimensional analysis leads to:-

$$\nu_s = F\varepsilon_s^{1/3}h^{4/3} \qquad (2)$$

where, **F** is a constant and h the grid scale. It is difficult to estimate ϵ_s so Smagorinsky (1963) modelled it using the large scale shear rate, (note, Kwak (1975) used vorticity instead of S_{ij}, and Schumann (1975) related υ_s to the subgrid energy);

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$$\nu_s = c^2 h^2 (2S_{ij}S_{ij})^{1/2}$$
$$S_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] \tag{3}$$

In this work, the fractal properties of the subgrid scale dissipation are used to estimate ϵ_s. Since a fractal description assumes similarity at all scales, and since, as we assume, only the largest length scale in the model relates to large scale quantities, it is expected that the accuracy of the calculation will depend less on the fineness of the filter used, enabling use of coarser meshes, an important practical consideration.

2.2 Fractals

Nature is not composed of perfect Euclidean figures; surfaces are pitted and grooved, coastlines are infinitely wavy and the borders of leaves consist of ever decreasing copies of the whole. The general concept of fractals is that parts of an object at different scales resemble the whole in some way, and that the 'fractal dimension' of the object is greater than its topological dimension (e.g. the two-scale Cantor set with exponents 0.3 and 0.7 has a fractal dimension of 2.36). Da Vinci (c.1490) first observed that the eddies in turbulent flow possess a comparable property of self-similarity. Their fractal dimension lies close to 2.36 (Meneveau et al.(1987)). It seems natural to employ fractal methods to model turbulence, utilizing the scaling properties of eddies, or more appropriately the transfer of turbulent energy and dissipation amongst them.

2.3 Scaling Properties

Since the Navier-Stokes equations given below,describe turbulent flow completely, the fractal nature of turbulence must be hidden in them.

$$\frac{D\vec{V}}{Dt} = -\nabla(p/\rho) + \nu\nabla^2\vec{V} \tag{4}$$

Frisch (1985) observed that a set of scaling transformations within the limits of $\eta <$ r, r' $\leq$ L and L $>> \eta$ preserve (4). L is the large scale imposed by external flow conditions and η is the Kolmogorov microscale below which turbulent kinetic energy is dissipated into heat by viscosity. The scaling transformations are:-

$$\begin{aligned} \vec{r}' &= \lambda\vec{r} \\ \vec{V}' &= \lambda^{\alpha/3}\vec{V} \\ t' &= \lambda^{1-\alpha/3}t \\ (p/\rho)' &= \lambda^{2\alpha/3}(p/\rho) \end{aligned} \tag{5}$$

where λ is a length-scale factor, and α is a scaling exponent. The dissipation ϵ under the same scaling transformations and at high Re (see Sreenivasan (1984)) is given by,

$$\epsilon_r \sim \frac{\delta v_r^3}{r} \tag{6}$$

where δv_r is a typical velocity difference over some length scale r. Then, ϵ_r rescales as:-
Using λ=r'/r and taking r'=L, leads to,

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$$\varepsilon_r' = \lambda^{\alpha-1}\varepsilon_r \tag{7}$$

$$\varepsilon_r = \varepsilon_L\left(\frac{r}{L}\right)^{\alpha-1} \tag{8}$$

Therefore, α can be expressed as a function of ϵ_r (where $\epsilon_r \neq 0$);

$$\alpha = \ln(\varepsilon_r/\varepsilon_L)/\ln(r/L) + 1 \tag{9}$$

Each of the quantities in equation (9) is governed by a probability distribution; the probability densities of ϵ_r and α are related by the following equation:-

$$P_\varepsilon(\varepsilon_r) = \frac{P_\alpha(\alpha)|d\alpha/d\varepsilon_r|}{P(\varepsilon_r \neq 0)} \tag{10}$$

The denominator dictates that at least part of the dissipation fractal at scale **r** belongs to the domain of size **r**. Equation (10) gives the probability density of ϵ_r, which is the total dissipation contained in a box of size **r**. From the α equation follows,

$$\frac{d\alpha}{d\varepsilon_r} = \frac{1}{\varepsilon_r \ln(r/L)} \tag{11}$$

To evaluate the R.H.S. p.d.f's we must use the multi-fractal framework.

2.4 Multifractals

Equation (9), can be rewritten as

$$\varepsilon_r = \left(\frac{\varepsilon_L}{L^{\alpha-1}}\right) r^{\alpha-1} \sim r^{\alpha-1} \tag{12}$$

Then, it may be assumed that α is a weight distributed on the fractal representing the areas of the flow containing dissipation, ϵ_r. In effect, α has then a multifractal distribution. We denote by $\mathbf{f}(\alpha)$ the fractal dimension of the set over which the scaling exponent takes a value between α and $\alpha+\mathbf{d}\alpha$. Meneveau et al.(1987), have shown how to derive $\mathbf{f}(\alpha)$, in terms of $\mathbf{D}_q$, a generalized dimension for a power law exponent **q**(see also Hentschel & Procaccia (1983) and Halsey et al. (1986)). The resulting analytic expressions are given below:-

$$\begin{aligned} f_d(\alpha) &= \alpha q-(q-1)(D_q-d+1)+d-1 \\ \alpha &= \frac{d}{dq}[(q-1)(D_q-d+1)] \end{aligned} \tag{13}$$

So, we can calculate α and $\mathbf{f}_d(\alpha)$ when $\mathbf{D}_q$ is known. For homogeneous fractals, $\mathbf{D}_q$ is in fact a constant, and does not depend on **q**. Meneveau et al. (1987), have determined the $\mathbf{f}(\alpha)$ vs α curve for a series of linear sections of the dissipation field (ie $\mathbf{d} = \mathbf{1}$) and for a wide range of flow situations. These included a laboratory boundary layer, the wake of a cylinder, grid turbulence and an atmospheric boundary layer. It has been found that for these and other flows studied by other investigators, that the $\mathbf{f}(\alpha)$ distribution is quasi-identical and so a single

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curve provides a very good approximation. The form of the $f(\alpha)$ curve, which represents the measured spectrum of the multifractal, suggests a parabola. The curve is not in fact parabolic; it has a maximum at $\alpha = 1.117$, and intersects the α-axis at $\alpha = 0.51$ and $\alpha = 1.78$ (see Figure 1).

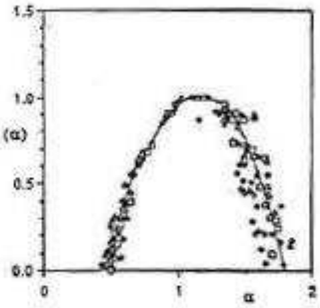

Figure 1. The $f(\alpha)$ curve (from Meneveau et al. (1989)

2.5 Probability density function of ϵ_r

With the $f(\alpha)$ curve known, the p.d.f's of equation (10), can be constructed. First, consider $P(\epsilon_r \neq 0)$; this is equal to the probability that a box of size r contains part of the multifractal. It can be written as a function of the multifractal dimension D_0 and r as,

$$P(\epsilon_r \neq 0) = c_1 (r/L)^{d-D_0} \tag{14}$$

Similarly, for $P(\alpha)$, considering that iso-α sets are fractals we can write,

$$P_\alpha(\alpha) = c_2 (r/L)^{d-f_d(\alpha)} \tag{15}$$

where c_1 and c_2 are constants. Combining the last two equations we get finally,

$$P_\epsilon(\epsilon_r) = \frac{C(r/L)^{D_0 - f_d[\ln(\epsilon_r/\epsilon_L)/\ln(r/L)+1]}}{\epsilon_r \left|\ln(r/L)\right|} \tag{16}$$

with a new constant C, replacing the previous two.

3. FLES SUBGRID MODEL

The biggest uncertainty in LES lies in estimating subgrid scale quantities from the macro-scale velocities. In the calculation of υ_s we need the value of ϵ_s at each computational node. In the previous section we saw how, using the multifractal formalism, a p.d.f. for dissipation at scale r can be calculated. The p.d.f. is used to estimate the dissipation in each CV cell, dependent upon the value of ϵ_L, the dissipation of large eddies present in the cell. In the absence of a transport equation for ϵ_L the expression due to Hinze (1975) has been used; then, as a function of the macro-scale velocities,

$$\epsilon_L = \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \tag{17}$$

From equation (17) we then get,

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$$\varepsilon_s = \int_{\varepsilon_{min}}^{\varepsilon_{max}} \frac{C(r/L)^{D_0 - f_s[\ln(\varepsilon_r/\varepsilon_L)/\ln(r/L) + 1]}}{|\ln(r/L)|} d\varepsilon_r \tag{18}$$

Assuming a total probability of 100%, the constant **C** may be evaluated. The limits of integration are obtained from the f-α function, given that α_{min} = **0.51** and α_{max} = **1.78**, and assuming negative values of f(α) are either unphysical, or represent rare events in the dissipation field. The volume average subgrid dissipation in a CV cell has thus been calculated. This is then used to estimate the subgrid scale viscosity.

$$\nu_S = F h^{4/3} \varepsilon_S^{1/3} \tag{19}$$

In this expression, derived from dimensional considerations, F is a constant to be determined and h the filter length related to the cell size. Finally,

$$\varepsilon_r = \varepsilon_L \ (r/l)^{\alpha - 1} \tag{20}$$

The integrals are evaluated using Simpson's method and a suitable step length.
To accommodate near-wall effects the Van Driest damping function is incorporated at present in the expression for ν_s, previously used in LES simulations by Quarini et al. (1979);

$$\nu_s = F \varepsilon_s^{1/3} (hD)^{4/3} \tag{21}$$

$$D = 1 - \exp[-(y^+/A^+)] \tag{22}$$

with y^+ the normalized distance to the nearest wall, A^+ = 25. The constant F is calculated by comparison with Smagorinsky and k-ε results in a duct; then, F=0.015. At first, this value appears to be one order of magnitude lower than that employed in Smagorinsky models. However, it should be recognised that to be comparable, F should be multiplied by $C^{1/3}$. As C$\approx$50 for the cases studied, the equivalent value of F is then close to 0.05.

4.CASES STUDIED

4.1 Test Case 1 - Turbulence decay in a duct

The case considered is a two-dimensional rectangular duct. The inlet boundary conditions are a plug velocity profile (Re=20000), to which have been added random fluctuations of about 10% of the bulk fluid velocity. No attempt has been made as yet, to account for the turbulence energy spectrum at the inlet. However, the fluctuation has been filtered, to remove frequencies which would otherwise fall below the subgrid scale limit chosen. For the enthalpy a similar method is employed with a plug profile hot fluid with a random variation entering a colder fluid. Gravity effects are modelled using a Boussinesq approximation which adds a momentum source term in the axial direction equal to,

$$G = -g\rho \frac{\beta}{c_p}(H_{ref} - H) \tag{23}$$

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$$\varepsilon_s = \int_{\varepsilon_{min}}^{\varepsilon_{max}} \frac{C(r/L)^{D_0 - f_\alpha[\ln(\varepsilon_r/\varepsilon_L)/\ln(r/L) + 1]}}{|\ln(r/L)|} d\varepsilon_r \tag{18}$$

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The subscript **ref** denotes a reference value and β is the volumetric coefficient of thermal expansion. Fluctuation amplitudes are compared for different gravity directions.

4.2 Test Case 2 - Flow over a backward-facing step

This is the study of the flow (Re=38000) in a duct with a 1.5:1 ratio sudden expansion. The inlet boundary conditions are a plug velocity profile as in the previous case and a short run-in is allowed for a turbulent velocity profile to develop as shown in figure 2. Of interest here are the correct treatment of the expanding shear-layer and prediction of the position of the reattachment zone. Studies on this case include the effect of not filtering the inlet boundary conditions and spatial grid sensitivity analysis. The length of time steps used in this study is 0.25% of the large eddy turnover time. A cartesian 93x60x10 grid was the finest grid used. The grid is equally spaced in the axial (x) and lateral (z) directions and concentrated near the walls in the vertical (y) direction to achieve sufficient resolution of the boundary layer. Symmetry conditions were assumed in the lateral (z) direction.

The model was attached to a CV-type general purpose CFD code using time-explicit time stepping and SIMPLE type pressure-velocity coupling. The calculations are initiated by superimposing a random velocity component to the inlet stream and then marching in time until statistically invariant conditions are reached (about 1400 timesteps). The results obtained contain mean and fluctuating velocities and temperatures, and in addition the subgrid quantities, effective viscosity, integral k (kinetic energy of turbulence) etc. The results, compared against experiments, conventional k-ϵ simulations and the standard Smagorinsky model show good agreement.

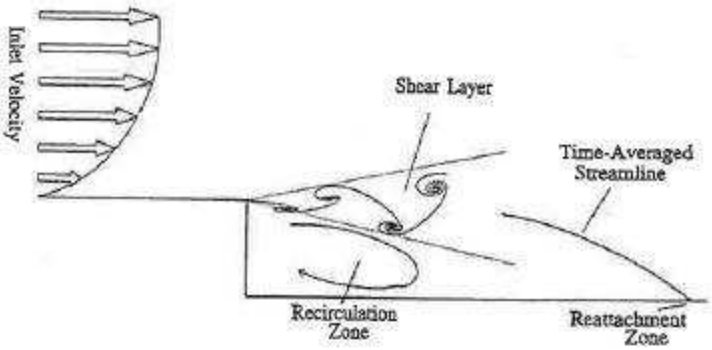

Figure 2: The bacward-facing step

5. NUMERICAL RESULTS

First, the duct flow with buoyancy (see also Dempsey et al.(1994)). Figure 3 shows the value of the subgrid viscosity in a section across the duct. As expected it is high close to the walls where turbulence is generated but falls away sharply at the wall and in the middle of the flow where most of the transport is at the large scales. In Figure 4, the effect of gravity on the axial velocity fluctuations is depicted. Axial fluctuations are enhanced when the flow is against the gravity vector, as in a rising thermal plume, and suppressed if the flow and gravity directions are the same, as expected in a stratifying situation. When there is no gravity, decay follows the theoretical grid decay curve.

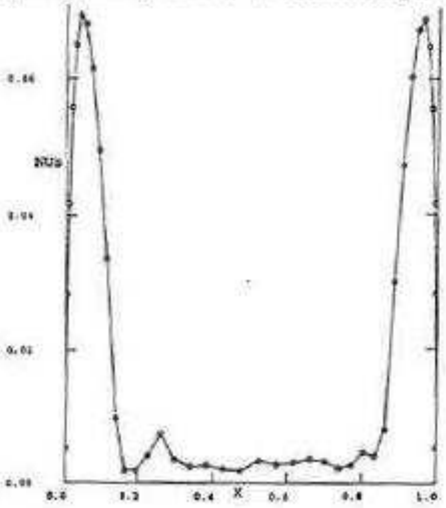

Figure 3: Subgrid viscosity across duct

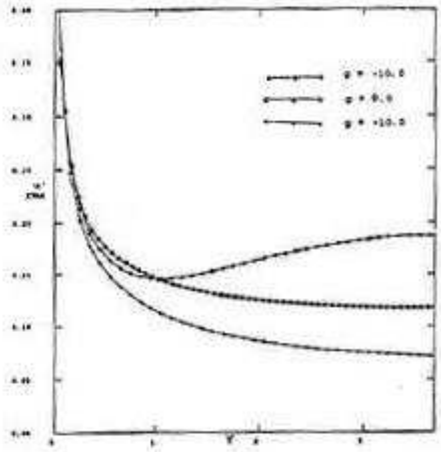

Figure 4: Effect of gravity on velocity fluctuations

Next, results from the backward facing step computation are shown. Figure 5, compares the time-averaged streamlines for the FLES model (a), and (b) the standard k-ε formulation. The k-ε model shows the basic recirculation zone but with a diminished length, 5.9h; the FLES model shows good agreement with a recirculation length of 7.0h (7.2h Ilegbusi (1979)) and also captures the counter rotating vortex at the bottom of the step and the small recirculation zone at the top of the duct.

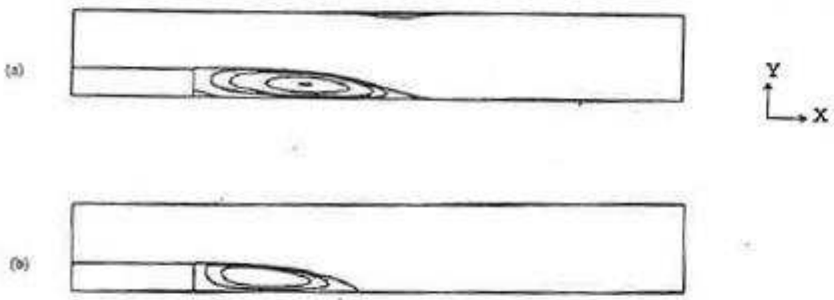

Figure 5: Recirculation behind the step (a) FLES; (b) k-ε

Velocity profiles of time-averaged and instantaneous axial velocity at different stations in the duct are given in Figure 6. The reattachment area appears to oscillate around the time averaged value. Figure 7, shows contours of various quantities of interest along the vertical midplane of the duct. Figure 7a, first shows the subgrid viscosity; maximum values occur in the shear layer, and downstream of the reattachment point. A peak at the top surface, marks the secondary separation region. Figure 7b, shows the fluctuating component of the axial

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velocity - not a subgrid quantity. Maximum amplitudes reach 27% of the mean inlet velocity. Maxima lie on either side of the reattachment point, again signalling oscillation of the shear layer.

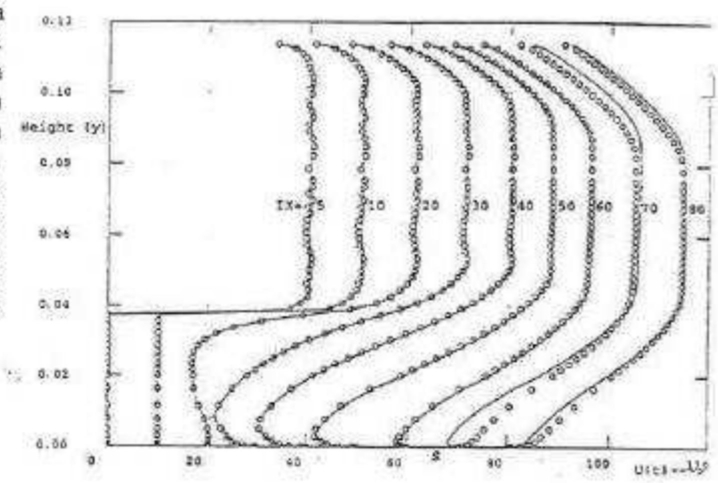

Figure 6: Mean and instantaneous velocity profiles

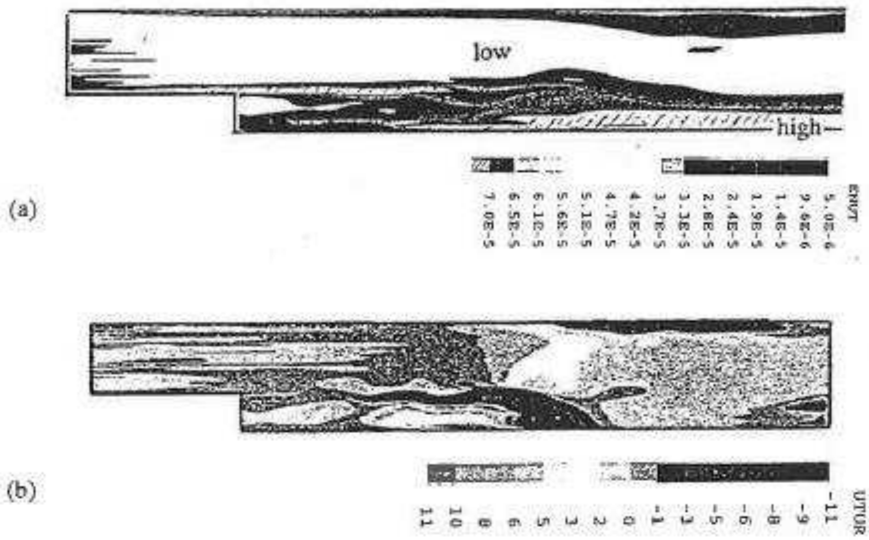

Figure 7: Mid-plane values,(a) Subgrid viscosity (b) U' fluctuations

6. CONCLUSIONS

This work demonstrates that by assuming similarity of scales in turbulent flows a fractal description of the subgrid eddy viscosity can be used. The resulting Fractal-LES scheme can be attached to standard CV type CFD codes, so that it can be readily accessed by engineers. Although much development is needed, the model has already demonstrated how, features of the flow which other models cannot easily resolve, i.e. the secondary recirculation zones in a backward facing step and the effects of gravity on non-isothermal flow can be easily captured.

Like all LES derivatives, the present model is expensive to use, compared to traditional two-equation models of turbulence. However it offers much more in terms of physical realism and it is simple to apply, having only one adjustable constant.

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