DEVELOPMENT AND APPLICATION OF THE DES k-ε TURBULENCE MODEL FOR FIRE SIMULATION

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ABSTRACT

In this paper, a Detached-Eddy Simulation (DES) method for turbulent flow prediction based on the k-ε model is developed and analyzed. The new method is then used to numerically simulate a typical forced convective problem. The results show that the new model, when compared with Large Eddy Simulation, gives solutions better agreed with the experimental data, while uses less grids. The model is also applied to a room fire case and the numerical results are compared with both LES results and experimental data.

Keywords: Detached-Eddy Simulation, turbulent model, forced convection, fire simulation

1. INTRODUCTION

For a long time, solving the Reynolds Averaged Navier-Stokes (RANS) equations has been the only practical method for industrial turbulent flow simulations. Recently, the Large Eddy Simulation (LES) is becoming popular in turbulence research community. However, the LES approach is computationally more expensive than RANS approaches. It is well-known that there is a strict demand of the size of computational grids for the LES approach. Especially near solid walls, the grids should be fine enough to resolve the turbulence structure, and the required number of grids will increase dramatically when the Reynolds number increase. At moderate Reynolds numbers, there are about 70 percent grids in the new-wall region, which takes up only 10 percent of the whole computational domain [1]. Therefore, it is still impractical to use the LES approach in industrial turbulent flow simulations at present and in the near future.

Spalart [2], after a comprehensive review of many turbulence simulation methods, reaches the conclusion that the most practical approach will be the Unsteady RANS (URANS) or RANS/LES hybrid model in the foreseeable future. The newly-developed Detached-Eddy Simulation (DES) method [3] in recent years is a promising example. Many applications show that DES is not only suitable for flows with massive separation, but also can be used as wall modeling method for LES [4]. This approach is quite efficient compared to LES while capturing the most important features of the flow.

In this paper, we develop a new DES approach based on k-ε model. To validate this method, it is then applied to simulate a typical forced convective problem. The emphasis of the present paper is to apply the proposed DES approach in fire simulations. We therefore use the present DES method to compute a room fire case. The numerical results are compared with LES results and experimental data.

2. DES APPROACH

The original DES method was proposed by Spalart [3] based on the Spalart-Allmaras one equation turbulence model. Travin et al. [5] later implemented DES method based on Menter's SST model [6] and gave a general definition of DES [7]: DES is a three-dimensional unsteady numerical solution using a single turbulence model, which functions as a subgrid-scale model in regions where the grid density is fine enough for the LES, and as a RANS model in regions where it is not. Bearing this general definition in mind, we propose a new DES approach based on the k-ε model, which has been widely used in fire simulations. Our hope is that it will combine the advantages of the well tested k-ε model in the boundary layers and the superior behavior of LES in the separated regions and the interior fields.

2.1 Standard k-ε Model

The standard k-ε model is as following:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho u_j k)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\mu+\frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}+G_k-\rho\varepsilon \tag{1}$$

$$\frac{\partial(\rho \varepsilon)}{\partial t}+\frac{\partial(\rho u_j \varepsilon)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}+\frac{\varepsilon}{k}\left(C_1 G_k-C_2\rho\varepsilon\right) \tag{2}$$

where, G_k is the production term of turbulence kinetics k.

$$G_k = \mu_T \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \quad (3)$$

The turbulent viscosity is defined by:

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon} \quad (4)$$

$C_1, C_2, C_\mu, \sigma_k$ and σ_ε are all model constants.

2.2 DES Approach Based on k-ε Model

The turbulent energy-contained length scale is:

$$l = \frac{k^{3/2}}{\varepsilon} \quad (5)$$

We replace the dissipation terms in the transport equation of k with the length scale above, that is,

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} + G_k - \rho \frac{k^{3/2}}{l} \quad (6)$$

with the ε equation unchanged.

According the philosophy of DES model, we change the definition of length scale as:

$$\bar{l} = \min\left(\frac{k^{3/2}}{\varepsilon}, C_{DES}\Delta\right) \quad (7)$$

where, C_{DES} is the model constant of DES approach, and is calibrated as 0.65 [8]; $\Delta = \max(\Delta_x, \Delta_y, \Delta_z)$ is the maximum size of local grid. We then replace the old definition in equation (6) with the new one. The k equation of DES approach is therefore:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} + G_k - \rho \frac{k^{3/2}}{\bar{l}} \quad (8)$$

The turbulent viscosity is then modified accordingly as:

$$\mu_T = \rho C_\mu k^{1/2} \bar{l} \quad (9)$$

2.3 Analysis of DES Approach

When $\frac{k^{3/2}}{\varepsilon} \le C_{DES}\Delta$, the DES approach we developed above is the standard k-ε model; when $\frac{k^{3/2}}{\varepsilon} > C_{DES}\Delta$, we consider the local equilibrium case. In this case, the production term of k equation, G_k is equal to the dissipative term, $\rho\varepsilon$, i.e.

$$G_k = \mu_T S = \rho \frac{k^{3/2}}{\tilde{l}}$$

where

$$S = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \text{ and } \tilde{l} = C_{DES}\Delta$$

Therefore we get $\mu_T = \rho(C_\mu^{3/4} C_{DES}\Delta)^2 \sqrt{S} \propto \sqrt{S}\Delta^2$, which is identical in form to the subgrid-scale Smargorinksy model in LES. We can see that, when the grid density is fine enough, the k-ε model based DES approach is the extension of Smagorinsky model with the non-equilibrium effect.

3. NUMERICAL ISSUES

We adopt the Fire Dynamics Simulator (FDS) software [9] of NIST as the Framework of our numerical simulations. FDS applies low Mach number approximation to solve compressible flows, and LES to simulate the turbulent flows in fires. The pressure equation is solved by Fast Fourier Transform (FFT) method. We replace the SGS model in FDS with the k-ε based DES model to construct a DES flow solver, and at the same time use the original FDS to calculate LES results for comparison.

The k and ε transport equations in k-ε based DES model can be written with a general form as:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi\mathbf{u}) = \nabla \cdot (\rho D_\phi \nabla\phi) + S_\phi \quad (10)$$

where, ϕ can be k or ε respectively, D_ϕ is the diffusion coefficient of ϕ; S_ϕ is the source term in ϕ equation.

The convection terms in equation (10) are discretized as:

$$\nabla \cdot (\rho\phi\mathbf{u})_{ijk} = \frac{(\rho\tilde{\phi}u)_{i+1/2,jk} - (\rho\tilde{\phi}u)_{i-1/2,jk}}{\Delta x} + \frac{(\rho\tilde{\phi}v)_{i,j+1/2,k} - (\rho\tilde{\phi}v)_{i,j-1/2,k}}{\Delta y} + \frac{(\rho\tilde{\phi}w)_{ij,k+1/2} - (\rho\tilde{\phi}w)_{ij,k-1/2}}{\Delta z} \quad (11)$$

where the $\tilde{\phi}_{i+1/2,jk}$ like terms are calculated with a second order upwind difference scheme with TVD properties:

$$\tilde{\phi}^{L}_{i+1/2,jk} = \phi_{ijk} + \frac{s^{i}_{ijk}}{4}\left[\left(1+\frac{s^{i}_{ijk}}{3}\right)\Delta^{i}_{ijk} + \left(1-\frac{s^{i}_{ijk}}{3}\right)\nabla^{i}_{ijk}\right] \quad (12)$$

$$\tilde{\phi}^{R}_{i+1/2,jk} = \phi_{i+1,jk} - \frac{s^{i}_{i+1,jk}}{4}\left[\left(1-\frac{s^{i}_{i+1,jk}}{3}\right)\Delta^{i}_{i+1,jk} + \left(1+\frac{s^{i}_{i+1,jk}}{3}\right)\nabla^{i}_{i+1,jk}\right] \quad (13)$$

$$\tilde{\phi}_{i+1/2,jk} = \begin{cases} \tilde{\phi}^{L}_{i+1/2,jk}, & if\ u_{i+1/2,jk} \geq 0 \\ \tilde{\phi}^{R}_{i+1/2,jk}, & otherwise \end{cases} \quad (14)$$

where, $\Delta^{i}_{ijk} = \phi_{i+1,jk} - \phi_{i,jk}$, $\nabla^{i}_{ijk} = \phi_{i,jk} - \phi_{i-1,jk}$; s_{ijk} is the Van Albada limiter:

$$s^{i}_{ijk} = \frac{2\Delta^{i}_{ijk}\nabla^{i}_{ijk} + \delta}{(\Delta^{i}_{ijk})^2 + (\nabla^{i}_{ijk})^2 + \delta} \quad (15)$$

where δ is a small positive number to prevent possible division by zero. All the superscripts i refer to the x direction; other directions can be inferred as well. The diffusion terms are discretized with second order central difference scheme.

Physical quantities are updated in time with a predictor-corrector scheme. The predictor and corrector steps are:

$$\frac{(\rho\phi)^{(n+1)_e}_{ijk} - (\rho\phi)^{n}_{ijk}}{\delta t} + \nabla\cdot(\rho\phi\mathbf{u})^{n}_{ijk} = [\nabla\cdot(\rho D_{\phi}\nabla\phi)]^{n}_{ijk} + S^{n}_{\phi} \quad (16)$$

and

$$\frac{(\rho\phi)^{(n+1)}_{ijk} - \frac{1}{2}\left((\rho\phi)^{n}_{ijk} + (\rho\phi)^{(n+1)e}_{ijk}\right)}{\delta t} + \nabla\cdot(\rho\phi\mathbf{u})^{(n+1)_e}_{ijk} = [\nabla\cdot(\rho D_{\phi}\nabla\phi)]^{(n+1)_e}_{ijk} + S^{(n+1)_e}_{\phi} \quad (17)$$

respectively. ϕ^{n} represents the value of ϕ at the time n; $\phi^{(n+1)_e}$ is the estimated value of ϕ at the time (n + 1). The whole method is second-order accuracy both in space and time. The source terms are linearized with negative coefficients to guarantee the convergence of numerical solutions.

4. RESULTS AND DISCUSSIONS

4.1 Forced Convection Case

To validate the k-ε model based DES approach we developed above, we apply it to a forced convective problem. Shown in Fig. 1 is the geometry: a single, isothermal, three-dimensional room. The inlet air enters the room along the ceiling with a velocity of 0.455 ms^{-1}. A passive exhaust is located near the floor on the opposite wall, with conditions specified such that there is no buildup of pressure in the enclosure. The initial conditions of simulations include no air motion, and a background temperature, density and pressure uniformly distributed in the room. Experimental measurements for this configuration were done by Restivo [10].

Simulations (both DES and LES) are conducted in conditions of various grid density, including 96 x 32 x 32, 96 x 48 x 48 and 96 x 64 x 64 in three directions respectively, to show the grid sensitivity of the simulation results. At the solid walls, the no-slip boundary conditions are applied. At the inlet, the turbulent kinetics and viscosity are prescribed, and at the outlet, we adopt the no gradient conditions. During DES simulations, wall function is used to calculate the turbulence quantities of grids adjacent to walls.

Illustrated in Fig. 2 is the comparison between numerical results and experimental data. All the data are in y = 1.5 m (middle of the room) plane, and simulations continued for a long enough time to eliminate the effect of initial conditions such that the results are steady as the experiment measurements.

Fig. 2(a) shows the u velocity results at x = 3 m (one third of the whole length of the room from the inlet) plotted with experimental data. As we can see, the DES simulation with coarser grids can already give results agreed with experimental data. Especially in the core flow region, the agreement is fairly good. On the other hand, the agreement in the boundary layer is not so good, but better than the LES simulation. LES simulation with finer grids cannot give as good results as DES even with coarse grids. In the core region, LES results agree with experimental data poorly, while better near ceiling, but the cost is that the velocity gradient at the outer side of jet is far steeper than experiment measurements, which is one of the causes for the poverty of LES agreement in core region.

Shown in Fig. 2(b) is the u velocity results at x = 6 m (two-thirds of the whole length of the room from inlet) plotted with experimental data. The same conclusion can be drawn that DES results outperform the LES results significantly.

Fig. 2(c) presents the u velocity results near ceiling (z = 2.916 m) plotted with experimental data. The numerical results are lower than experimental data as a whole. This is due to that the size of the inlet is so small that the grid cells use to describe it are few [11]. We increase the inlet height to fit the grid. To maintain the correct flow rate, the velocity at the inlet is therefore reduced. To improve the numerical results of both LES and DES, more grids near the ceiling are needed.

Fig. 2(d) shows the u velocity results near floor (z = 0.084 m) plotted against measures experimentally. When finer grids are used, the DES results are better at the left side than when coarser grids are adopted. But in the middle and near right side the discrepancy in DES results and experimental data is greater and DES is approaching LES, while LES results have obvious difference from the measures experimentally in the middle.

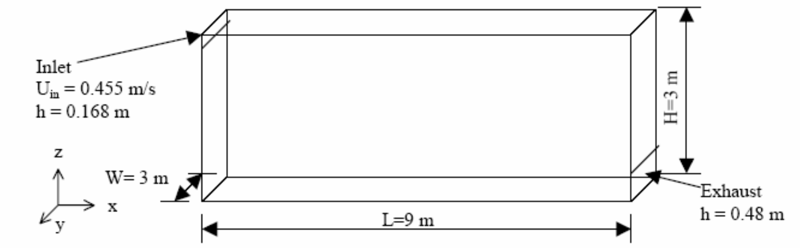
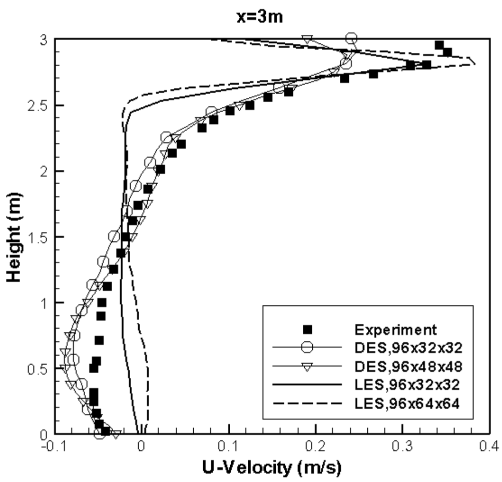
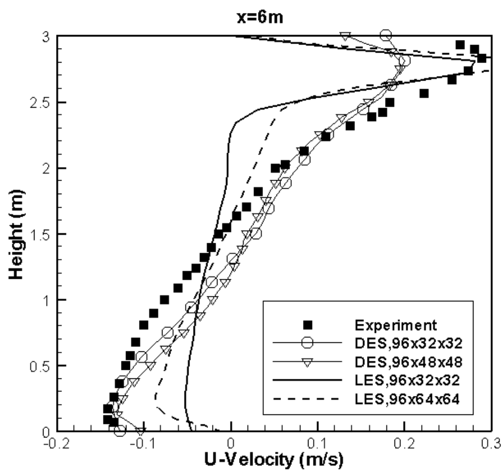


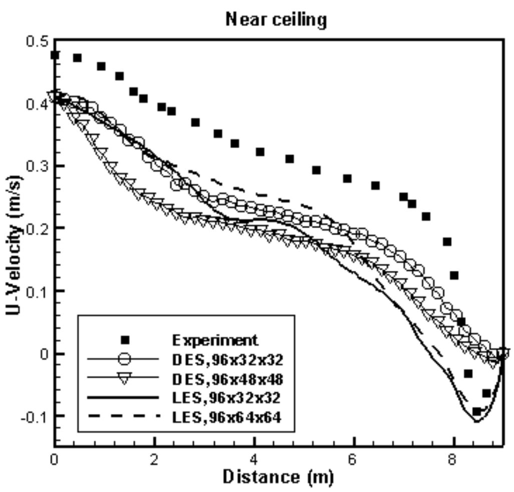
Fig. 1: Geometry for the forced convection case



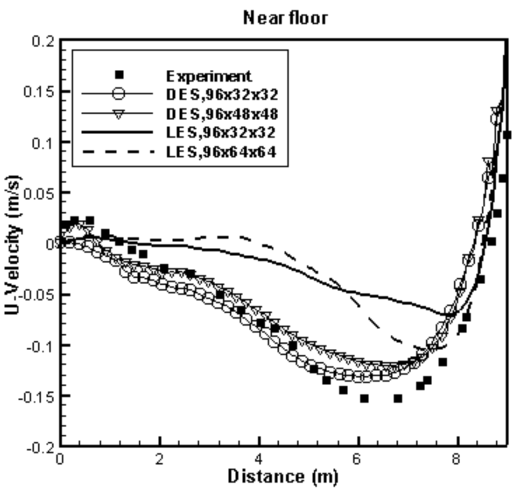
(a) x = 3 m



(b) x = 6 m



(c) z = 2.916 m



(d) z = 0.084 m

Fig. 2: Comparison of numerical results and experimental data

A fact is worth our notice. Emmerich et al. [12] studied this case using LES and their results show that, different Smagorinsky SGS model constants C_s have great impact on the numerical results. Our LES simulation included no optimization for C_s, so our results are worse than Emmerich's. However, this will not overrule our conclusion above, even compared to the best results of Emmerich et al. The reason is that, we adopt uniform computational grid. So for LES, the grid size is generally not fine enough to resolve flow structure at boundary, consequently the error is comparatively great, which inversely affects the flow parameters of interior grids and makes LES results poor. The DES approach, nevertheless, is less sensitive to grids than LES. Thus DES approach can obtain considerably good results when coarse grids are used.

4.2 Room Fire Case

To examine the performance of the DES k-ε model for fire case, it is applied to a room fire benchmark case. In this case, the buoyancy induced turbulence production terms are added to the DES k-ε model to account for the buoyancy effects. Steckler et al. [13] conducted this compartment fire experiment and it has been a test case for fire simulation package developers since. The non-spreading fire was created using a centrally located 62.9 kW methane burner with a diameter of 0.3 m. The compartment room is 2.8 m x 2.8 m in plane and 2.18 m in height with a doorway centrally located in one of the walls measuring 0.74 m wide by 1.83 m high, as shown in Fig. 3. The walls and ceiling were 0.1 m thick and they were covered with a ceramic fiber insulation board to establish near steady state conditions within 30 minutes. An average outdoor temperature of 302 K was assumed. The floor, ceiling and walls were assumed as adiabatic and perfect radiative reflectors.

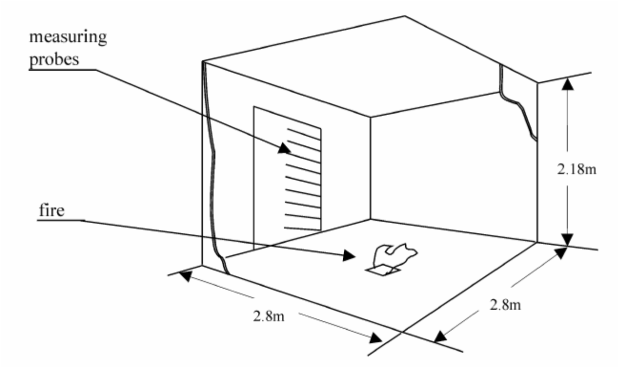
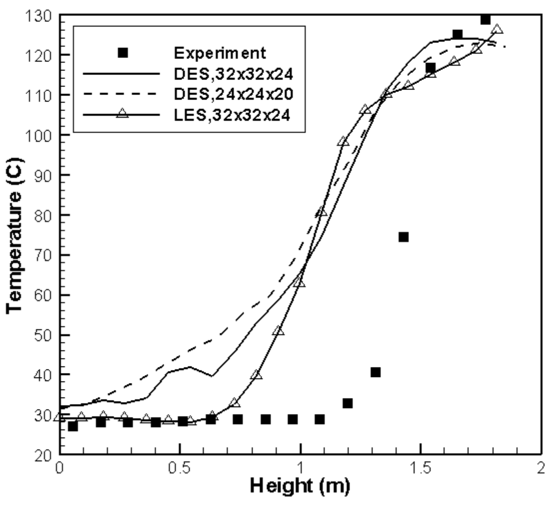
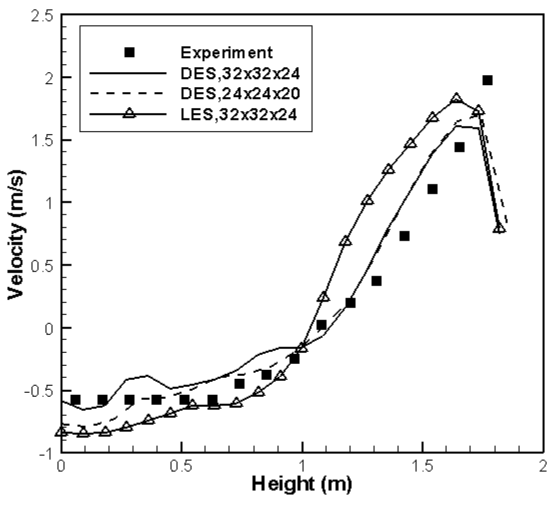


Fig. 3: Sketch of the Steckler's room fire

Simulation of this fire case was carried out with 24 x 24 x 20 and 32 x 32 x 24 grids. The numerical results (DES and LES) at the middle of the opening are plotted in Fig. 4 against the experimental data for comparison. It is seen that the DES method can give fairly good results for velocity profile that is significantly better than that predicted with LES. For the temperature distributions, both DES and LES give rather poor results. It seems that the LES predicts the thermal stratification slightly better than DES.



(a) Temperature distribution



(b) Velocity distribution

Fig. 4: Results of the Steckler's room fire case

The reason for the failure of both the DES and LES models to predict the temperature profile can be complicated. As we all know, the prediction of velocity and temperature near the fire source is very hard. The turbulent combustion models used in FDS may be inadequate to account for the complicated interaction between fire plume and air entrainment at the middle of the room height.

5. CONCLUSION

Starting from the general definition of Detached-eddy Simulation, we develop a new DES approach based on k-ε model and apply it to a typical forced convection case for validation. Comparison between numerical results of DES and LES and experimental data shows that, DES approach obtains results well agreed with experimental data using less grids, and captures important feature of flows with separation.

The application of this method to fire case is investigated by simulation of a room fire. The results are fairly good as to the velocity, while the temperature distribution is not. The reason for this is uncertain yet. But the inadequate of modeling for turbulence-chemistry interaction may be the main contributor. This issue needs further study.

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