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Large eddy simulation of a medium-scale methanol pool fire using the extended eddy dissipation concept

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ABSTRACT

The eddy dissipation concept (EDC) is extended to the large eddy simulation (LES) framework following the same logic of the turbulent energy cascade as originally proposed by Magnussen but taking into account the distinctive roles of the sub-grid scale turbulence. A series of structure levels are assumed to exist under the filter width "Δ" in the turbulent energy cascade which spans from the Kolmogorov to the integral scale. The total kinetic energy and its dissipation rate are expressed using the sub-grid scale (SGS) quantities. Assuming infinitely fast chemistry, the filtered reaction rate in the EDC is controlled by the turbulent mixing rate between the fine structures at Kolmogorov scales and the surrounding fluids. The newly extended EDC was implemented in the open source FireFOAM solver, and large eddy simulation of a 30.5 cm diameter methanol pool fire was performed using this solver. Reasonable agreement is achieved by comparing the predicted heat release rate, radiative fraction, velocity and its fluctuation, temperature and its fluctuation, turbulent heat flux, SGS and total dissipation rate, SGS and total kinetic energy, time scales, and length scales with the corresponding experimental data.

1. Introduction

The eddy dissipation concept (EDC) originally developed by Magnussen [1,2] assumes that chemical reactions take place in fine structures which have similar magnitudes as the Kolmogorov scales and that the reaction rate is determined from the turbulent mixing rate between the fine structures and surrounding fluids. Thus, the turbulent effect on combustion is embedded in the reaction rate of EDC. The EDC is well established for the Reynolds Averaged Navier–Stokes (RANS) approach, but its extension to the large eddy simulation (LES) framework has been problematic partly because the eddy characteristic time scale cannot be easily determined in LES. Fureby and co-workers [3,4] proposed a procedure to calculate the turbulent reaction rate by directly replacing the total kinetic energy and its dissipation rate with the sub-grid scale (SGS) properties. This approach has been adopted by some commercial CFD codes like FLUENT [5]. However, it was reported that the predicted reaction rate is strongly dependent on grid size [3]. This was thought to be likely caused by the replacement of the total kinetic energy with the SGS kinetic energy. Note that in LES the SGS kinetic energy represents the unresolved turbulent energy to be modeled and this energy should be much less than the total kinetic energy.

In the present study, a new approach will be developed to extend the EDC from RANS to LES, from which the characteristic time scales and length scales are derived. Numerical simulation of a 30.5 cm diameter methanol pool fire will be performed to evaluate the development.

2. Extention of the eddy dissipation concept

2.1. Turbulent energy cascade

The essence of the EDC assumes that a stepwise turbulent energy cascade exists from the mean flow down to the Kolmogorov scale, and the heat generation resulting from the dissipation of turbulence energy mainly occurs on the small scales where production and dissipation balance [6]. This assumption is believed to be independent of the chosen turbulence models, either RANS or LES, but it does neglect backscatter and upscale transfer which exist in real physics but would only have marginal influence on the present applications where the interests are more focused on the mean and fluctuating flow variables and radiative heat emissions from fires. Given the fact that the filter width of LES generally falls between the Kolmogorov and integral length scale, we assume that there is a series of structure levels below the filter width Δ in the stepwise turbulent cascade as shown in Fig. 1. As properties on this 'Δ' level can be determined directly from a SGS turbulence model, we can derive expressions for the characteristic variables on other

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Nomenclature

C	constant
c_p	specific heat capacity
g	gravitational acceleration
k	kinetic energy
L	length scale
L_f	flame height
MW_i	molar weight of the species i
p_i	partial pressure of the species i
Q	heat release rate
q	dissipation heat
s	stoichiometric oxygen–fuel ratio
T	temperature
u	velocity scale
W	mechanical energy
Y_i	species mass fraction for the species i

Greeks symbols

γ	mass fraction of the fine structures
Δ	LES filter width
ε	dissipation rate
κ	local absorption coefficient
ρ	density
σ	Stefan–Boltzmann constant
χ	reacting fraction of the fine structures
υ	kinematic viscosity
ω	strain rate
$\overline{\omega}_i$	filtered reaction rate of the species i

Subscripts

fu	fuel
N_2	nitrogen
n	n-th structure level
O_2	oxygen
SGS	sub-grid scale

structure levels using these SGS quantities. Thus, the total kinetic energy and its dissipation rate may be calculated from the SGS quantities following assumptions made in the original EDC [6].

In Fig. 1, u_n, L_n and ω_n represent the velocity scale, length scale and strain rate on the n-th structure level. Following Ertesvåg and Magnussen [6], the strain rate ω_n is assumed to be equal to $2\omega_{n-1}$ with regard to the relationship between two adjacent structure levels. q_n represents thermal energy resulting from dissipation on each level while W_n stands for the sum of mechanical energy on all subsequent levels. On the n-th level, W_n and q_n may be expressed as [6].

$$W_n = \frac{3}{2} C_{D1} \omega_n u_n^2 \tag{1}$$

$$q_n = C_{D2} \upsilon \omega_n^2 \tag{2}$$

$$\omega_n = \frac{u_n}{L_n} \tag{3}$$

$$\omega_n = 2\omega_{n-1} \tag{4}$$

where υ is the molecular kinematic viscosity, C_{D1} and C_{D2} are model coefficients. According to Eqs. (2) and (4),

$$q_n = 4q_{n-1} \tag{5}$$

The total dissipation rate of the kinetic energy may be modeled as [6]

$$\varepsilon = q' + q'' + \cdots + q_n + q_{n+1} + \cdots + q_{SGS} + q_1 + \cdots + q^* \tag{6}$$

Substituting Eq. (5) into Eq. (6) and then applying the series theory,

$$4q^* - q' = 3\varepsilon \tag{7}$$

Similarly, W_{SGS} on the 'Δ' level may be expressed as

$$W_{SGS} = q_{SGS} + q_1 + q_2 + \cdots + q^* \tag{8}$$

Substituting Eq. (5) into Eq. (8),

$$4q^* - q_{SGS} = 3W_{SGS} \tag{9}$$

And subtracting Eq. (9) from Eq. (7),

$$\varepsilon = W_{SGS} + \frac{1}{3} q_{SGS} - \frac{1}{3} q' \tag{10}$$

q' can be considered as negligible since the dissipation into heat mainly takes place on the small scales rather than the integral scale. According to Eqs. (1)–(3), Eq. (10) can be re-written as

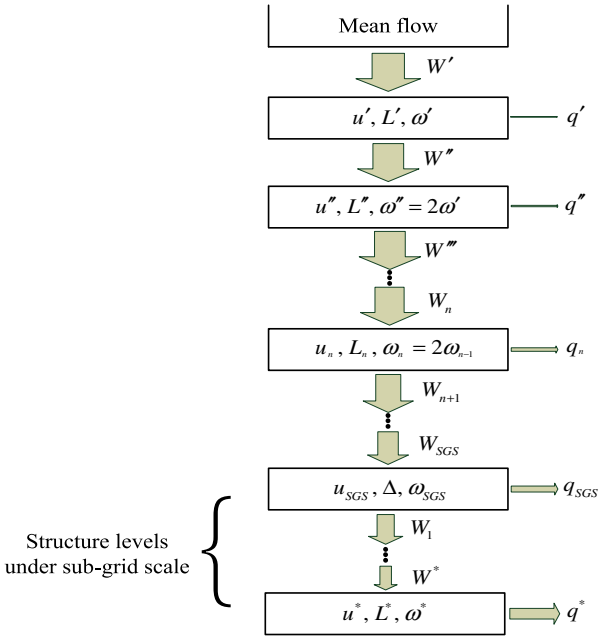

Fig. 1. The turbulent energy cascade in the LES framework.

$$\varepsilon \approx W_{SGS} + \frac{1}{3} q_{SGS} = \frac{3}{2} C_{D1} \frac{u_{SGS}^3}{\Delta} + \frac{1}{3} C_{D2} \upsilon \frac{u_{SGS}^2}{\Delta^2} \tag{11}$$

u_{SGS} is estimated to be $\sqrt{\frac{2}{3} k_{SGS}}$, where k_{SGS} is SGS kinetic energy obtained from a LES model such as sub-grid kinetic energy model [7]. Therefore,

$$\varepsilon \approx \sqrt{\frac{2}{3}} C_{D1} \frac{k_{SGS}^{3/2}}{\Delta} + \frac{2}{9} C_{D2} \upsilon \frac{k_{SGS}}{\Delta^2} \tag{12}$$

Based on the energy conservation on all the structure levels,

$$W' = \varepsilon = \frac{3}{2} C_{D1} \frac{(u')^3}{L'} \tag{13}$$

where L' is the integral length scale. u' is calculated from $\sqrt{\frac{2}{3} k}$, and k is the total kinetic energy. Thus,