# The Extension of Eddy Dissipation Concept in the Framework of Large Eddy Simulation and the Subsequent Modification

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#### **1** Introduction

The eddy dissipation concept (EDC) originally developed by Magnussen assumes that chemical reaction takes place in fine structures which have the same magnitude of the Kolmogorov scales. Distinct from the eddy dissipation model [1], it allows for some consideration of detailed chemistry for both premixed and non-premixed flames. A comprehensive introduction of its theoretical foundation, mainly associated with turbulence energy cascade, is included in [2, 3].

The EDC is well established for Reynolds Averaged Navier-Stokes (RANS) equations, but there still exists a gap for its extension to the large eddy simulation (LES) framework since the eddy characteristic time scale cannot be easily determined in LES. Fureby and co-workers [4, 5] proposed a procedure to calculate the turbulent mixing rate by directly replacing the total kinetic energy and its dissipation rate with the sub-grid scale (SGS) properties, which is widely used in the combustion community such as the commercial CFD code FLUENT. It was reported that the reaction rate is strongly dependent on grid size [4], which is attributed to be the replacement of the total kinetic energy with the SGS kinetic energy. In LES, the SGS kinetic energy represents the unresolved turbulent energy and needs to be modeled during the simulation. The SGS energy is normally much less than the total kinetic energy and varies with the grid resolution. Recently, Zhou et al. [6] found that the EDC fails to give satisfactory predictions in comparison with other combustion models. Panjwani and Ertesvag [7] investigated the possibility to extend the EDC in the LES framework, still using the same approach as Fureby and co-workers to compute the reaction rate. They reported numerical instability which was thought to be caused by the non-physical distribution of the mass fraction occupied by the fine structures. Yaga [8] presented a promising alternative to account for the turbulent reaction rate with Kolmogorov time scale, where the total dissipation rate is linked to the strain rate, and good agreement was achieved for temperature and species profiles in the combustor.

In this paper, the reaction rate of EDC is derived according to turbulent energy cascade concept in the LES framework, and the formula for the mass fraction of fine structures is improved accordingly. Predictions were conducted for a 30.5cm methanol pool fire to evaluate the extended EDC.

# 2 Extension of the EDC to LES framework and the subsequent modification

In the EDC, a stepwise turbulent energy cascade [2] is supposed to take place from mean flow down to Kolmogorov scale, and the heat generation resulting from the dissipation of turbulence energy is assumed to mainly occur on the small scales where production and dissipation balance. This assumption is believed to be independent of the chosen turbulence models, for instance RANS or LES. The filter width of LES is between Kolmogorov length scale and integral length scale, and hence SGS properties such as SGS kinetic energy and filter width are at one of the structure levels of the stepwise turbulent cascade as shown in Fig.1.



Fig. 1 stepwise turbulent energy cascade from large scales to small scales in the LES framework

In Fig.1,  $u_n$ ,  $L_n$ , and  $\omega_n$  represent the velocity scale, length scale and strain rate scale on the *n*-th structure level respectively, and in this study  $\omega_n$  is still assumed to be  $2\omega_{n-1}$  according to the orginal EDC.  $W_n$  stands for the sum of mechanical energy at the subsequent steps, while  $q_n$  represents thermal energy resulting from the dissipation. For the *n*-th level,  $W_n$  and  $q_n$  can be expressed as [2],

$$W_{n} = \frac{3}{2} C_{D1} \omega_{n} u_{n}^{2}$$
 (1)

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

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

Note that  $\nu$  is the molecular kinematic viscosity. Since properties on the ' $\Delta$ ' filter level can be determined directly from a SGS turbulence model, characteristic scales on other levels are likely to be derived accordingly. Therefore integral turbulence parameters such as the dissipation rate might be described on the SGS basis. In this study, the dissipation rate is modeled as follows based on the formulation of Magnussen [2]

$$\mathcal{E} = q' + q'' + \dots + q_n + q_{n+1} + \dots + q_{SGS} + q_1 + \dots + q^*$$
(4)

Given by the relationship of  $\omega_n$  between two adjacent structure levels,

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

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Thus,

$$4q^* - q' = 3\varepsilon \tag{6}$$

q' is negligible since the transfer from the mechanical energy to the heat mainly occurs on the small scales, then

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

For the structure levels under the filter width,  $W_{SGS}$  is calculated according to the energy conservation,

$$W_{SGS} = q_{SGS} + q_1 + q_2 + \dots + q^*$$
(8)

$$q_1 = 4q_{SGS}, \quad q_2 = 4q_1, \quad \cdots$$
 (9)

Assuming there are N structure levels under the sub-grid scale,

$$W_{SGS} = q_{SGS} \left( 1 + 4 + 4^2 + \dots + 4^N \right) = \frac{1}{3} q_{SGS} \left( 4^{N+1} - 1 \right) = \frac{1}{3} \left( 4q^* - q_{SGS} \right)$$
(10)

Substituting Eqs. (1)-(3) and (7) into Eq. (10),

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

 $u_{SGS}$  is of the magnitude of  $\sqrt{\frac{2}{3}k_{SGS}}$ , where  $k_{SGS}$  is SGS kinetic energy and provided by a LES model. Therefore,

$$\varepsilon = \sqrt{\frac{2}{3}} C_{D1} \frac{k_{SGS}^{3/2}}{\Delta} + \frac{2}{9} C_{D2} v \frac{k_{SGS}}{\Delta^2}$$
(12)

For the last level (i.e. fine structures),  $W^*$  is equal to  $q^*$  in terms of energy conservation, so the characteristic scales can be obtained with the combination of Eq. (7),

$$L^{*} = \frac{2}{3} \left( \frac{3C_{D2}^{3}}{C_{D1}^{2}} \right)^{1/4} \left( \frac{v^{3}}{\varepsilon} \right)^{1/4}$$
(13)

$$u^{*} = \left(\frac{C_{D2}}{3C_{D1}^{2}}\right)^{1/4} (\upsilon \varepsilon)^{1/4}$$
(14)

In this study,  $u^*$  and  $L^*$  are supposed to be the same as Kolmogorov scales, implying that  $C_{D1}=0.5$  and  $C_{D2}=0.75$ . These two constants differ from the original EDC, where the values are calculated from the turbulence viscosity of k- $\varepsilon$  model [2].

The ratio of the mass transfer between the fine structures and surroundings and the fine-structure mass is calculated using the same formula as in the original EDC [2],

$$\dot{m}^* = \frac{2u^*}{L^*} = \left(\frac{3}{C_{D2}}\right)^{1/2} \left(\frac{\varepsilon}{v}\right)^{1/2}$$
(15)

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For the ratio of the fine structure mass to the total mass in the original EDC, Magnussen presented two different formulations [2, 3] linked to the relationship of characteristic velocity scales, based on the early studies of turbulence intermittency by Corrsin [9] and Tennekes [10], respectively. Here this variable is calculated according to subsequent studies of Frisch and Kolmogorov [11] based on experimental findings,

$$\gamma = \left(\frac{L^*}{L_I}\right)^{\alpha} \tag{16}$$

where  $L_l$  is the integral length scale, and  $\alpha$  is a constant of 0.2 [12]. Moreover, this treatment of  $\gamma$  is expected to avoid the applicability of total kinetic energy which cannot be explicitly calculated in a LES. The integral length scale is often related to a typical geometric characteristic of a given scenario. In the fire community, this scale is likely to be proportional to the characteristic plume structure scale [13, 14], widely used to measure the grid resolution for fire plumes simulations. It can be expressed as,

$$L_{I} = bD, \quad D = \left(\frac{\dot{Q}}{\rho_{\infty}c_{p}T_{\infty}\sqrt{g}}\right)^{2/5}$$
(17)

*b* is a constant, set as 0.1 in this work;  $\dot{Q}$  is the heat release rate;  $\rho_{\infty}$  is the ambient density;  $T_{\infty}$  is the ambient temperature;  $c_p$  is the specific heat; *g* is the gravity acceleration.

It is assumed in the original EDC that the finite reaction takes place in the fine structures which can be regarded as a well stirred reactor, and the reaction rate is mainly controlled by the turbulent mixing among these fine structures. The filtered reaction rate in a LES can be thus given by,

$$\tilde{R}_{i} = \bar{\rho}\dot{m}^{*}\frac{\mathcal{H}}{1-\mathcal{H}}\left(\tilde{Y}_{i}-Y_{i}^{*}\right)$$
(18)

 $Y_i^*$  is the mass fraction for the specie *i* in the fine structures, and  $\chi$  is the reacting mass fraction of fine structures, which has been improved in our earlier work [15] to tackle the ignition problem of the original EDC [2, 3]. For instance, the filtered reaction rate of fuel with the assumption of fast chemistry for the non-premixed combustion can be expressed as

$$\tilde{R}_{fu} = \overline{\rho} \dot{m}^* \frac{\mathcal{H}}{1 - \mathcal{H}} \min\left(\tilde{Y}_{fu}, \frac{\tilde{Y}_{O_2}}{s}\right)$$
(19)

where *s* is the stoichiometric oxygen to fuel ratio.

#### **3** Results and discussion

The 30.5cm methanol pool fire tested by Weckman and Strong [16] is used to evaluate the extended and modified EDC and its implementation into the FireFOAM solver [17]. Fast chemistry is assumed for the combustion and b was selected to be 0.1. The one equation eddy viscosity model [18] was employed to take into account the SGS kinetic energy. A cylindrical computational domain was chosen to be 90cm in diameter, 180cm in height with non-uniform meshes, and a grid sensitivity study was performed to ensure the results presented below are grid independent. The methanol feeding rate is 1.07g/s giving 24.6kW heat release rate. The inlet temperature was set as 350K, slightly greater than the evaporation temperature of methanol. Radiation loss was considered with the assumption of optically thin flame.

Figures 2-3 show the comparison of the predicted temperature and axial velocity distributions with the experimental data at four different heights. Reasonable good agreement is achieved for the temperature profiles. At the lower locations (say 2cm) close to the fuel pan, the current model under-predicts the temperature by around 200K, especially near the pool centerline. This can be attributed to the under-prediction of the mixing rate by the EDC because turbulence is not fully developed in this region. Predicted axial velocity profiles agree well with the measurements at all the elevations.



Fig. 2 Comparison of predicted and measured temperature at different heights



Fig. 3 Comparison of predicted and measured axial velocity at different heights

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### 4 Conclusions

The EDC based on RANS has been extended to the LES framework in this paper, according to the turbulent energy cascade. A 30.5cm methanol pool fire simulation has been conducted to test the extended and modified model. Reasonably good agreement has been achieved for temperature and velocity. More scenarios are needed to further validate this extension.

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