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A MODEL FOR FLAME EXTINCTION IN TURBULENT FLOW

S. Byggstøyl
Researcher, SINTEF Avd. 15
and
B.F. Magnussen
Professor, Engineering Thermodynamics
The Norwegian Institute of Technology
Division of Thermodynamics
N-7034 Trondheim-NTH, Norway

ABSTRACT

In this paper a model for local extinction in turbulent flow is developed The model is based on the Eddy Dissipation Concept (EDC) for chemical reaction in turbulent flow developed by Magnussen (1981)[1]. A review of this concept is included in the paper. The (EDC) is a reactor concept which is unique in that it takes into account the intermittent behaviour of the smallscale structures of turbulence, as well as the effect of the fine structures on the chemical reactions. Both fast and slow chemical reactions can be treated simultanelously and consequently the extinction process. In this paper the extinction is assumed to take place in the fine structure. The lift-off and blow-out conditions for turbulent diffusion flames are calculated and compared with experimental data. The turbulent flame propangation velocity is also discussed with regards to the same concept.

NOMENCLATURE

c_i	concentration (kg/m^3)
c_p	specific heat
D	nozzle diameter
F	flatness factor
F	characteristic fine structure flatness factor
ΔH_R	reaction enthalpy difference
k	turbulence kinetic energy
L*	characteristic length scale of fine structures
L'	characteristic turbulence length scale mixing length
L", L^n	characteristic turbulence length at different structure level
$\dot{m}$	exchange rate of mass with fine structures
Re_λ	turbulence Reynolds number
r	stoichiometric oxygen requirement to burn 1 kg fuel
T	temperature (K)
ΔT	excess temperature of reacting fine structures
U_B	turbulent flame velocity
$\bar{U}$	mean flow velocity
u*	characteristic velocity of fine structures
u'	turbulence velocity
u",u^n	characteristic turbulence velocity at different structure level
x	axial coordinate
Y	fractional conversion parameter
y	lateral coordinate
ρ	density
ε	rate of dissipation of turbulence kinetic energy
μ_t	effective turbulent viscocity
ν	kinematic viscosity
γ^*	intermittency factor
γ_λ	mass fraction occupied by fine structures
	mass fraction occupied by fine structures regions
τ^*	time scale for the fine structure
τ_{ch}	chemical time scale
τ_λ	time scale for the fine structure regions
τ_M	bulk mixing timescale

INTRODUCTION

Local extinction in a practical turbulent combustion situation can influence important combustion characteristics like stability, noise generation, flame propangation, fuel consumption and heat transfer. These characteristics are of main importance for the performance and operation of combustion engines, combustion chambers, flare burners and fire fighting equipment.

From a fundamental point of view the extinction characteristics of chemical reactions in turbulent flow can give some new information about the geometry and the dynamics of the small scale turbulent structure and the interaction between the structure and chemical reactions which is some of the main problems in turbulence. The classical way to treat extinction phenomena is to apply Karlovitz-Kovasnays criterium resently used in a turbulent combustion situation by Chomiak (1982)[2]. Turbulent structure models have been developed and used by Lockwood and Megahed (1978)[3] and Tabaczynski (1981)[4]. Common for these models is that the chemical kinetical properties of the fluid is expressed through the laminar flame speed.

Recently Peters (1982)[5] treated the extinction process in turbulent flow by considering the quenching of diffusive flamelets where both the intermittant behaviour of turbulence and chemical kinetics were taken into account.

REVIEW OF EDC

Chemical reactions take place when reactants are mixed at molecular scale at sufficiently high temperature[1]. In turbulent flow the reactant consumption is strongly dependent on the molecular mixing. It is known that the microscale processes which are decisive for the molecular mixing as well as dissipation of turbulence energy into heat are severely intermittent i.e. concentrated in isolated regions whose entire volume is a small fraction of the volume of the fluid.

These regions are occupied by fine structures whose dimensions are small in one or two directions, however not in the third. These fine structures are believed to be vortex tubes, sheets or slabs whose characteristic dimensions are of the same magnitude as the Kolmogorov microscale. [6,7,8,9,10]

The fine structures are responsible for the dissipation of turbulence into heat. Within these structures one can therefore assume that reactants will be mixed at molecular scale. These structures thus create the reaction space for non-uniformly distributed reactants.

In a modelling context one can assume that the reactants are homogeneously mixed within the fine structures. Thus, in order to be able to treat the reactions within this space, it is necessary to know the reaction volume and the mass transfer rate between the structures and the surrounding fluid.

The following describes a concept for treating chemical reactions in turbulent flow which include basic features of the preceeding.

Turbulence energy dissipation

In turbulent flow energy from the mean flow is transferred through the bigger eddies to the fine structures where mechanical energy is dissipated into heat. This process is schematically described in Fig. 1.

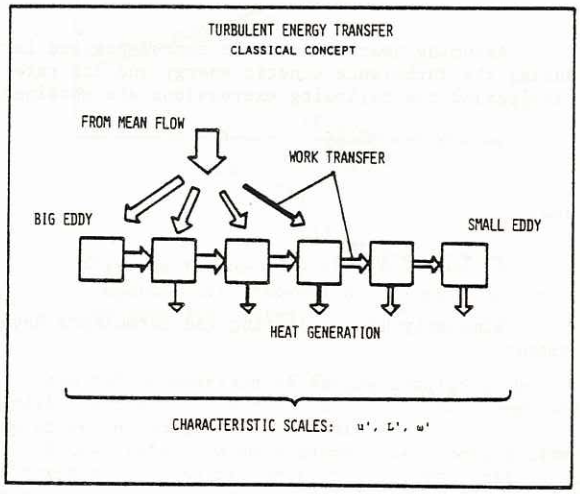

Fig. 1. Turbulent energy transfer

In general, high Reynolds number turbulent flow will consist of a spectrum of eddies of different sizes. Mechanical energy is mainly transferred between neighbouring eddy structures as indicated in Fig. 1. For the same reason the main production of turbulence kinetic energy will be performed by the interactions between bigger eddies and the mean flow.

The dissipation of kinetic energy into heat, which is due to work done by molecular forces on the turbulence eddies, on the other hand mainly takes place in the smallest eddies.

Important turbulent flow characteristics can for nearly isotropic turbulence be related to a turbulence velocity, u', and a turbulent length, L'. These quantities are linked to each other through the turbulent eddy velocity:

$$\nu_t = u' \cdot L' \tag{1}$$

Modelling interstructural energy transfer

Figure 2 schematically illustrates a model for the transfer of mechanical energy from bigger to smaller turbulent structures[11].

The first structure level represents the whole spectrum of turbulence which in an ordinary way is characterized by a turbulence velocity, u', a length scale, L', and vorticity, or characteristic strain rate

$$\omega' = u'/L' \tag{2}$$

The rate of dissipation can for this level be expressed by

$$\varepsilon' = \zeta^2 (12 \frac{u'}{L'} \cdot u''^2 + 15 \cdot \nu (\frac{u'}{L'})^2) \tag{3}$$

where ζ is a numerical constant.

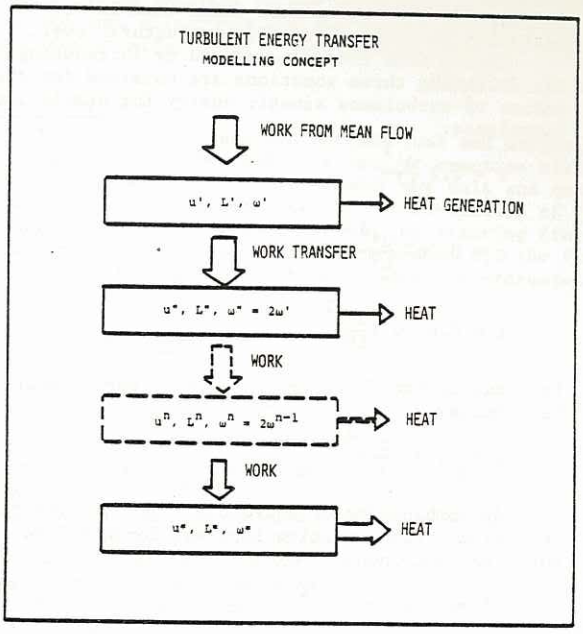

Fig. 2. A modelling concept for transfer of energy from bigger to smaller turbulent structures

The next structures level represent part of the turbulence spectrum characterized by a vorticity

$$\omega'' = 2\omega' \tag{4}$$

velocity, u", and length scale, L". The transfer of energy from the first level to the second level is expressed by

$$w' = \zeta^2 \, 12 \, \frac{u'}{L'} \, u''^2 \tag{5}$$

Similarly the transfer of energy from the second to the third level where

$$\omega''' = \omega'' \tag{6}$$

is expressed

$$w'' = \zeta^2 \, 12 \, \frac{u''}{L''} \cdot u'''^2 \tag{7}$$

The part which is directly dissipated into heat is expressed

$$q'' = \zeta^2 \cdot 15\nu (\frac{u''}{L''})^2 \tag{8}$$

The turbulence energy ballance for the second structure level is concequently given by

$$\zeta^2 \, 12 \, \frac{u'}{L'} \, u''^2 = \zeta^2 (12 \, \frac{u''}{L''} \cdot u'''^2 + 15 \cdot \nu (\frac{u''}{L''})^2) \tag{9}$$

This sequence of turbulence structure levels can be continued down to a level where all the produced turbulence kinetic energy is dissipated into heat. This is the fine structure level characterized by, u*, L*, and ω*.

The turbulence energy transferred to the fine structure is expressed by

$$w^* = \zeta^2 \cdot 6 \, \frac{u^*}{L^*} \cdot u^{*2} \tag{10}$$

and the dissipation by

$$q^* = \zeta^2 \cdot 15\nu \, (\frac{u^*}{L^*})^2 \tag{11}$$

According to this model nearly no dissipation of energy into heat takes place at the highest structure

level. Similarly it can be shown that 3/4 of the dissipation takes place at the fine structure level.

Taking this into account and by introducing $\zeta = 0.18$ the following three equations are obtained for the dissipation of turbulence kinetic energy for nearly isotropic turbulence:

$$\varepsilon = 0.2 \frac{u'^3}{L'} \tag{12}$$

$$\varepsilon = 0.267 \frac{u^{*3}}{L^*} \tag{13}$$

$$\varepsilon = 0.67 \nu \left(\frac{u^*}{L^*}\right)^2 \tag{14}$$

Introducing the Taylor microscale a fourth equation is obtained

$$\varepsilon = 15 \nu \left(\frac{u'}{\lambda}\right)^2 \tag{15}$$

By combination of equations (13) and (14) the following characteristics (scales) for the fine structures are obtained

$$u^* = 1.74 \, (\varepsilon \cdot \nu)^{1/4} \tag{16}$$

and

$$L^* = 1.43 \, \nu^{3/4} / \varepsilon^{1/4} \tag{17}$$

where u^* is the mass average fine structure velocity. The scales are closely related to the Kolmogorov scales.

The fine structures

The tendency towards strong dissipation intermittency in high Reynolds number turbulence was discovered by Batchelor and Townsend[11], and then studied from two points of view; different statistical models for the cascade of energy starting from a hypothesis of local invariance or selfsimilarities between motions of different scales, and then by consideration of hydrodynamic vorticity production due to stretching of vortex lines.

It can be concluded that the smallscale structures who are responsible for the main part of the dissipation are generated in a very localized fashion. It is assumed that these structures consist typically of large thin vortex sheets, ribbons of vorticity of vortex tubes of random extension folded or tangeled throughout the flow (Fig. 3).

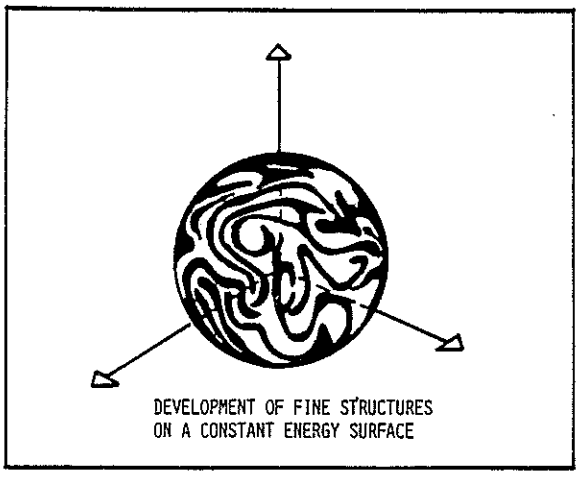

Fig. 3. Schematic illustration of fine structures developed on a constant energy surface

The fine structures are localized in certain fine structure regions whose linear dimensions are considerably larger than the fine structures therein[10]. These regions appear in the highly stained regions between the bigger eddies.

Modelling characteristics of the fine structures

It is assumed that the mass fraction occupied by the fine structures, on the basis of consideration of the energy transfer to these structures (eqs. 12 and 13) can be expressed by

$$\gamma^* = \left(\frac{u^*}{u'}\right)^3 \tag{18}$$

If it is assumed that the fine structures are localized in nearly constant energy regions, then the mass fraction occupied by the fine structure regions can be expressed by

$$\gamma^* = \gamma_\lambda \cdot \left(\frac{u^*}{u'}\right)^2 \tag{19}$$

giving the following expression

$$\gamma_\lambda = \frac{u^*}{u'} \tag{20}$$

Assuming nearly isotropic turbulence and introducing the turbulence kinetic energy and its rate of dissipation the following expressions are obtained:

$$\gamma^* = 9.7 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2}\right)^{3/4} \tag{21}$$

and

$$\gamma_\lambda = 2.13 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2}\right)^{1/4} \tag{22}$$

Similarly by introducing the turbulence Reynolds number

$$\gamma^* = 40.2 \cdot Re_\lambda^{-3/2} \tag{23}$$

and

$$\gamma_\lambda = 3.42 \cdot Re_\lambda^{-1/2} \tag{24}$$

Kuo and Corrsin[8] have given some results for the flatness factor of $\partial u/\partial t$ as a function of Re_λ (Fig. 5). In order to compare the above results with these results an empirical expression has been developed for the relationship between the flatness factor and the intermittency factor:

$$F_M = 1.5 \cdot (1 + 1/\gamma) \tag{25}$$

Figure 4 shows a comparison between some experimental results[10] and the given empirical expression.

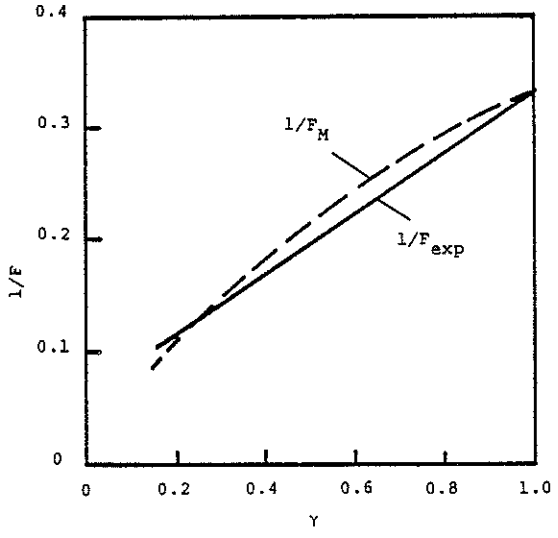

Fig. 4. Comparison between experimental results and empirical expression for the flatness factor as a function of the intermittency factor.

When eq. (25) is applied the following expression for the flatness factor for the fine structures is obtained.

$$F_\lambda = 1.5 + 0.44 \cdot Re_\lambda^{0.5} \tag{26}$$

Equation (26) is compared with the experimental results of Kuo and Corrsin[9] in Fig. 5.

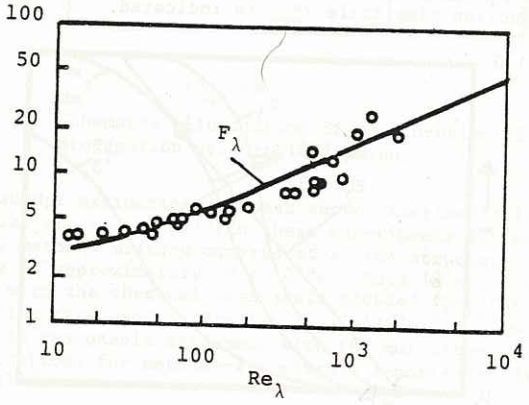

Fig. 5. Flatness factor of $\partial u/\partial t$ as a function of Re_λ compared with theoretical flatness factor for the fine structures.

From this comparison it can be concluded that the overall features of the physics seem to have been taken care of by the suggested expressions.

On the basis of simple geometrical considerations the transfer of mass per unit of fluid and unit of time between the fine structures and the surrounding can be expressed as follows

$$\dot{m} = 2 \cdot \frac{u^*}{L^*} \cdot \gamma^* \quad (1/s) \tag{27}$$

Expressed by k and ε for nearly isotropic turbulence eq. (27) turns into

$$\dot{m} = 23.6 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2}\right)^{1/4} \cdot \frac{\varepsilon}{k} \quad (1/s) \tag{28}$$

Molecular mixing and reaction processes

The rate of molecular mixing is determined by the rate of mixing between the fine structures and the surrounding fluid.

The mean mass transfer rate between a certain fraction, χ, of the fine structures and the rest of the fluid, R_i, can for a certain specie, i, be expressed as follows:

$$R_i = \dot{m} \cdot \chi \cdot \left(\frac{c_i^o}{\rho^o} - \frac{c_i^*}{\rho^*}\right) \tag{29}$$

where * and ^{o} refer to conditions in the fine structures and the surrounding.

The mass transfer rate can also be expressed per unit volume in the fine structure fraction, χ, as

$$R_i^* = \frac{\dot{m} \cdot \rho^*}{\gamma^*} \cdot \left(\frac{c_i^o}{\rho^o} - \frac{c_i^*}{\rho^*}\right) \tag{30}$$

Finally, the concentration of a specie, i, in the fraction, χ, of the fine structures and in the surrounding is related to the mean concentration by:

$$\frac{\bar{c}_i}{\bar{\rho}} = \frac{c_i^*}{\rho^*} \cdot \gamma^* \cdot \chi + \frac{c_i^o}{\rho^o} \cdot (1 - \gamma^* \cdot \chi) \tag{31}$$

It is now possible to put up balance equations for reacting fine structures and the surrounding fluid including chemical kinetic rate expressions.

Combustion rates

If the rate of reaction between fuel and oxygen is considered infinitely fast, the rate of reaction will be limited by the mass transfer between the bulk and the fine structures. In this case the concentration of fuel or oxygen will be very small within the reacting fine structures. If the reaction took place in all the fine structures, the rate of combustion would be expressed by:

$$R_{fu} = \dot{m} \cdot \frac{\bar{c}_{min}}{1-\gamma^*} \tag{32}$$

where $\bar{c}_{min}$ is the smallest of $\bar{c}_{fu}$ and $\bar{c}_{O_2}/r_{fu}$, where $\bar{c}_{fu}$ and $\bar{c}_{O_2}$ are the local mean concentrations of fuel and oxygen, and r_{fu} the stoichiometric oxygen requirement.

Not all the fine structures will be sufficiently heated to react. This is obviously the case in combustion of premixed gases where both fuel and oxygen are present in the fine structures.

The fraction of the fine structures which reacts can be assumed proportional to the ratio between the local concentration of reacted fuel and the total fuel concentration:

$$\chi = \frac{\bar{c}_{pr}/((1+r_{fu}) \cdot \gamma_\lambda}{\bar{c}_{pr}/(1+r_{fu}) + \bar{c}_{fu}} \tag{33}$$

where $\bar{c}_{pr}$ is the local mean concentration of reaction products. Equation (33) implies the assumption that the reaction products are kept within the fine structure region until a concentration is reached which yields χ equal to unity.

By combination of equations (32) and (33) the following general equation is obtained for the rate of combustion at infinite reaction rate between fuel and oxygen:

$$R_{fu} = \dot{m} \cdot \frac{\chi}{1 - \gamma^* \chi} \cdot \bar{c}_{min} \tag{34}$$

The reacting fine structures under these conditions will have a temperature, ΔT, in excess of the local mean temperature:

$$\Delta T = \frac{\Delta H_R \cdot \bar{c}_{min}}{\bar{\rho} \cdot c_p} \tag{35}$$

where ΔH_R is the heat of reaction and c_p the local specific heat capacity. The temperature, T*, of the reacting fine structures is consequently:

$$T^* = \bar{T} + \Delta T \tag{36}$$

and the surrounding temperature:

$$T^o = \bar{T} - \Delta T \cdot \frac{\gamma^* \cdot \chi}{1 - \gamma^* \cdot \chi} \tag{37}$$

where $\bar{T}$ is the local time mean temperature.

Chemical controlled reaction rate

On the basis of the precious there can be defined characteristic mixing time scales:

The bulk mixing time scale

$$\tau_M = 1/\dot{m} \tag{38}$$

The fine structure time scales

$$\tau^* = \gamma^*/\dot{m} \tag{39}$$

$$\tau_\lambda = \gamma_\lambda/\dot{m} \tag{40}$$

These time scales can be compared with chemical kinetic time scales in order to establish whether the reaction is mixing or chemical controlled, and even established criteria for extinction of flames.

MODELING FLAME EXTINCTION AND TURBULENT FLAME PROPAGATION ACCORDING TO THE EDC

Extinction

According to the previous concept heat and mass balance including chemical kinetics can easily be set up for the fine structures and the surrounding fluid. Consequently, knowing the chemical kinetics, a criterium for the extinction of the fine structures can be obtained. When a typical timescale for the combustion reaction is small compared to τ^* the fuel consumption is independent of chemical kinetics and is a purely hydrodynamic problem. However when the residence time becomes smaller than a typical chemical time scale the reaction will not be completed in the fine structure and the fuel consumption is strongly influenced by chemical kinetics. As the residence time decreases extinction will finally occur.

The chemical time scale, however, is not a uniquely defined quantity. Many different expressions can be found in the literature describing the various steps in the reaction process. In addition it is very difficult to find relevant data for different fuels.

When studying turbulent extinction a common substitute for the lacking chemical kinetic data has been time scales based on the laminar flame propagation behaviour of the mixture[3,4]. These time scales are, however, more dependent on the diffusive properties of the fluid than the chemical kinetics. Another time scale that has been used is the chemical induction time or ignition delay time. This time scale is usually measured in shock tube experiments where the reaction starts from the very low radical concentration level of the unheated gases. This is not the case in flames and other reacting systems where there exists a source of free radicals somewhere in the system. Here the induction time is much shorter. In a typical turbulent combustion situation it is believed that radicals are already present in the regions where the fine structures are located. When it is further assumed that the internal mixing inside the fine structures are fast then the fine structures can be considered as a well stirred reactor.

On the basis of the previous the fractional conversion parameter for the reactor is defined as (cfr. Fig. 6)

$$Y = \frac{c_{fu}^{o} - c_{fu}^{*}\frac{\rho^{o}}{\rho^{*}}}{c_{fu}^{o}} \tag{41}$$

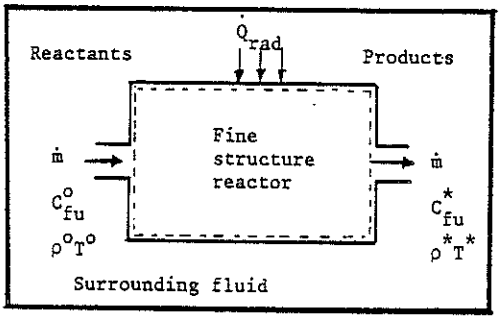

Fig. 6. Schematic illustration of a reacting fine structure

For a one step irreversible reaction the mass and heat balance for the fine structure can be expressed as

$$Y = \frac{R_{fu}^{*} \cdot \tau^{*}}{c_{fu}^{o}} \frac{\rho^{o}}{\rho^{*}} \tag{42}$$

$$Y = \frac{c_p (T^* - T^o)\rho^o}{\Delta H_R \, c_{fu}^o} \tag{43}$$

where the fine structure is considered to be adiabatic and the specific heat of the fluid is assumed to be constant. The extinction time scale can then be found from eq. (42) and (43) according to Fig. 7, where the extinction time scale τ^*_{ext} is indicated.

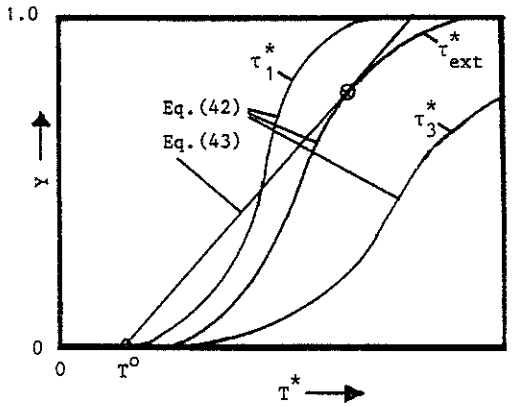

Fig. 7. Schematic illustration of Extinction in the fine structure $\tau_1^* > \tau_{ext}^* > \tau_3^*$

Turbulent flame propagation

The propagation of a plane flame in turbulent flow can be expressed by

$$U_B \frac{\partial c_{fu}}{\partial x} = \frac{\nu_T}{\sigma} \frac{\partial^2 c_{fu}}{\partial \chi^2} + R_{fu} \tag{44}$$

where U_B is the turbulent flame propagation velocity, ν_T is the turbulent viscosity and σ is the turbulent Schmidt number. With R_{fu} expressed according to Eq. (34), the only physical meaningful solution to Eq. (44) reads

$$U_B = 2 \left(\frac{\dot{m}\nu_t}{\gamma_\lambda \sigma} \right)^{1/2} \tag{45}$$

By introducing the turbulent viscosity from the k-ε-model this transforms into

$$U_B = 2 \sqrt{\frac{k}{\sigma}} \tag{46}$$

In a typical shear flow situation $k \cong u'^2$ and $\sigma \cong 1$. This gives a turbulent flame propagation velocity

$$U_B \cong 2u' \tag{47}$$

This is generally in relatively close agreement with the experimental data collected by Bradley et.a. (1981)[14]

When the fine structure-time scale τ^* is reduced to the same magnitude as the chemical time scale, the turbulent flame speed is reduced due to local extinction in the fine structures. At a critical value of the fine structure-time scale the flame will be quenched by the turbulence. This leads to the following general qualitativ relation for the turbulent flame speed:

$$\frac{U_B}{u'} = f(\tau_{ch}^*/\tau^*) \tag{48}$$

Due to the strong interaction between T^* and τ_{ch}^*/τ^*, the flame quenching appears like a catastrophy as indicated in fig. 8.

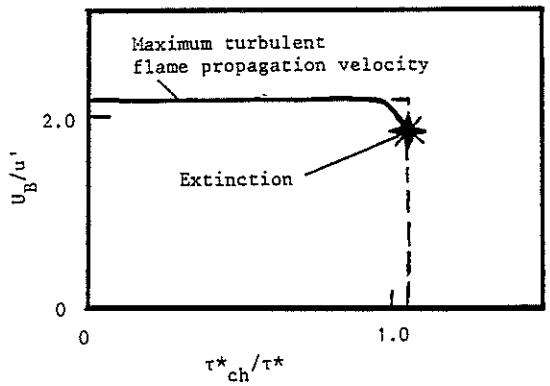

Fig. 8. Schematic illustration of the turbulent flame propagation velocity variation.

The abrupt extinction has been shown experimentally by Chomiak et. al. (1982)[3]. In these experiments extinction for a methane mixture occured at a fine structure time scale of approximately $\tau^* \approx 10^{-4}$s This in close agreement with the chemical time scale deduced from the global reaction rate used by Bradley et.al.(1976)[15,16] and is also in reasonable agreement with the multistep kinetic calculations for methane-air mixture reported by Martenay (1970)[17].

Lift-off and blow-off of turbulent diffusion flames

According to the extinction model and the result for the turbulent flame speed a lifted diffusion flame will be stabilized near the position on the stochiometric contour where the fine structure time scale equals the chemical time scale. The reason why the stabilization point is located at or near the stochiometric contour is that the reaction rate has its maximum near this contour. This is shown in fig. 9. where also some calculated fine structure time scales at the stabilization points are indicated. By gradually increasing the exit velocity the stabilization point moves further downstreams. This continues until the stabilization point is at a position where the mean flow velocity is nearly equal to the maximum flame propagation velocity, then the flame is blown-off. This is shown in Fig. 9 where also some calculated fine structure timescales at the stabilization points are inducated.

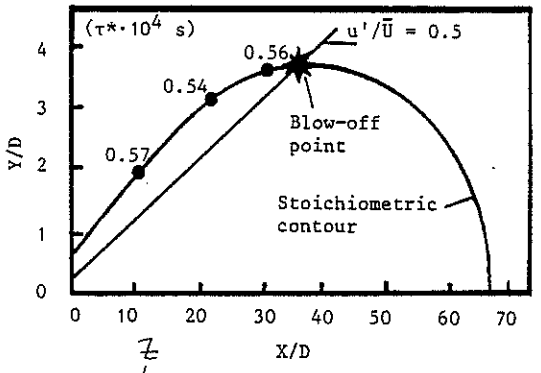

Fig. 9. Localisation of lift-off and blow-off points for a round free jet. Experimental data from Horch (18) for D = 0.01 m.

The extinction model has been tested by performing numerical calculations of the jet flow based on the k-ε model of turbulence and then extracting the quenching time scales by comparison with the experimental data of Horch (1978)[18].

Figure 10 shows a comparison between experimental and predicted lift-off heights. The predictions have been based on a constant fine structure timescale, $\tau^* = 0.56 \cdot 10^{-4}$ s.

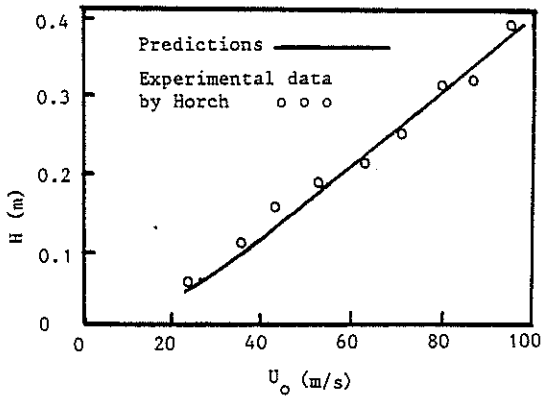

Fig. 10. Comparison between experimental and predicted lift-off heights.

For a constant nozzle diameter the fine structure timescale at the stabilization points was nearly constant as shown both in Figs. 9 and 10, indicating that the fine structures are of main importance in the extinction process. The time scale did, however, decrease with increasing diameter, as indicated in Table 1.

Table 1. Mean structure time scale at the stabilisation point for different nozzle diameters.

D (mm)	4	6	8	10
$\tau^* \cdot 10^4$(s)	1.18	0.80	0.67	0.56

We assume that this diameter effect is due to radiative heat transfer between the fine structures at the flame stabilization point and its surroundings. This effect will tend to increase the fine structure temperatures and consequently reduce the extinction time scales for increased nozzle diameter. As such this effect can readily be handled by the described concept. At the blow-off point the ratio of a typical turbulence velocity to the mean flow velocity was nearly equal to $u'/\bar{U} \approx 0.5$. This is shown in Fig. 9 and table 2.

Table 2. Turbulence intensity at blow-off point for different nozzle diameters.

D (mm)	4	6	8	10
$u'/\bar{U}$	0.51	0.47	0.49	0.48

According to the previous, the mean velocity is nearly equal to the maximum turbulent flame propagation velocity at the blow-off point.

CONCLUSIONS

The previous have shown that extinction processes in turbulent combustion can be treated by the eddy dissipation concept (EDC) of Magnussen. Predictions deduced from the proposed extinction model compares well with experimental data.

The flame stabilization point for lifted diffusion flames is located at the stoichiometric contour and at positions where the fine structure mixing time scale τ^* is approximately equal to the chemical time scale τ^*_{ch}.

An expression for the turbulent flame propagation velocity is deduced from the EDC. This expression gives results which are in close agreement with experimental data. It is shown that blow-off for turbulent diffusion flames occurs at a point where the maximum turbulent flame propagation velocity is equal to the mean flow velocity.

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