ON THE STRUCTURE OF TURBULENCE AND A GENERALIZED EDDY DISSIPATION CONCEPT FOR CHEMICAL REACTION IN TURBULENT FLOW

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ON THE STRUCTURE OF TURBULENCE AND A GENERALIZED EDDY DISSIPATION CONCEPT FOR CHEMICAL REACTION IN TURBULENT FLOW

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Abstract

The paper discusses an eddy dissipation concept for treating chemical reactions in turbulent flow. An essential feature of this concept is that it takes into account the fact that the molecular mixing between reactants, which is associated with the dissipation of turbulence, takes place in concentrated, isolated regions that occupy only a small fraction of the total volume of the fluid.

The mass fraction occupied by the dissipative regions, as well as the mass transfer rate between these regions and the surrounding fluid, are determined from turbulence theory thus providing new general fluid mechanical information for the solution of reaction problems. This enables fast and accurate calculations of turbulent combustion phenomena.

The treatment of fast and slow chemical reactions in turbulent flow is discussed in relation to this concept. Comparison is made with experimental data.

Nomenclature

c_i	concentration (kg/m^3)
c_p	specific heat
D	nozzle diameter
F	Flatness factor
F_λ	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^*	characteristic velocity of fine structures
u'	turbulence velocity
u'', u^n	characteristic turbulence velocity at different structure level
x	axial coordinate
y	lattera1 coordinate
ρ	density
ε	rate of dissipation of turbulence kinetic energy
μ_t	effective turbulent viscocity
ν	kinematic viscocity
γ	intermittency factor
γ^*	mass fraction occupied by fine structures
γ_λ	mass fraction occupied by fine structure regions
χ	fraction of fine structures reacting
λ	Taylor microscale
ω^n	u^n/L^n
τ	characteristic time scale

Superscripts

-	time-mean value
*	fine structure
o	surrounding fluid
n	number of structure level

Subscripts

fu	fuel
i	specie
pr	product

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Introduction

Chemical reactions taking place in turbulent flow are strongly influenced by flow parameters. In general an inhomogeneous structure of the appearance of the various reacting species will develope as a concequence of the chemical reactions 1,2.

Due to the complexity of turbulent flow and the chemical kinetics, as well as the interaction between turbulence and the chemical reaction, it is impossible to perform a rigorous treatment. Consequently the interaction between the turbulence and the chemical kinetics must be modelled.

Basic considerations

Chemical reactions take place when reactants are mixed at molecular scale at sufficiently high temperature. 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.[3,4,5,6,7]

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 fine 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.

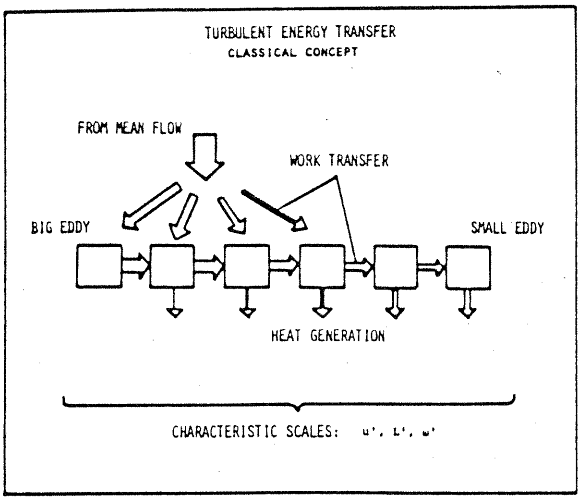

Fig. 1. Turbulent energy transfer.

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:

$$\nu_t = u' \cdot L' \qquad (1)$$

Modelling interstructural energy transfer

Figure 2 schematically illustrates a model for the transfer of mechanical energy from bigger to smaller turbulent structures[8].

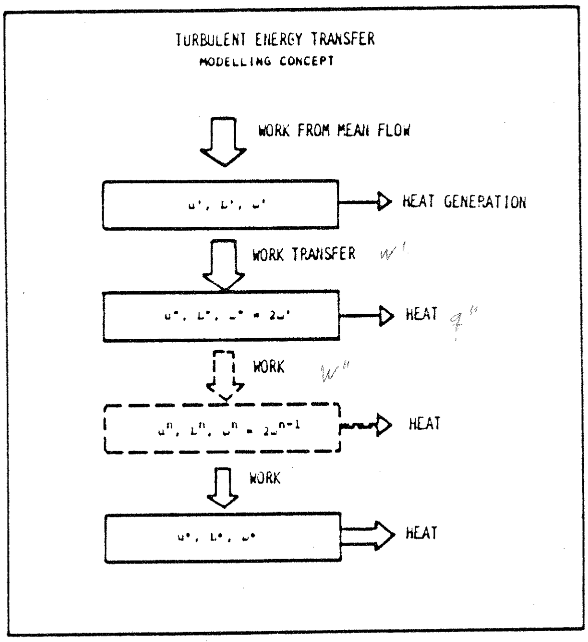

Fig. 2. A modelling concept for transfer of energy from bigger to smaller turbulent structures.

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

$$\omega' = u'/L' \qquad (2)$$

The rate of dissipation can for this level be expressed by

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

where ζ is a numerical constant.

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

$$\omega'' = 2\omega' \qquad (4)$$

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

$$w' = \zeta^2 12 \frac{u'}{L'} u''^2 \qquad (5)$$

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

$$\omega''' = 2\omega'' \qquad (6)$$

is expressed

$$w'' = \zeta^2 12 \frac{u''}{L''} \cdot u'''^2 \qquad (7)$$

The part which is directly dissipated into heat is expressed

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

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

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

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 transfered to the fine structure by

$$w^* = \zeta^2 \cdot 6 \frac{u^*}{L^*} \cdot u^{*2} \qquad (10)$$

and the dissipation by

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

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:

$$\varepsilon = 0.2 \frac{u'^3}{L'} \qquad (12)$$

$$\varepsilon = 0.267 \frac{u^{*3}}{L^*} \qquad (13)$$

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

Introducing the Taylor microscale a fourth equation is obtained

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

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

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

and

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

where u^* is the mass average fine structure velocity. These 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[9], 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 or vortex tubes of random extension folded or tangeled throughout the flow (fig. 3).

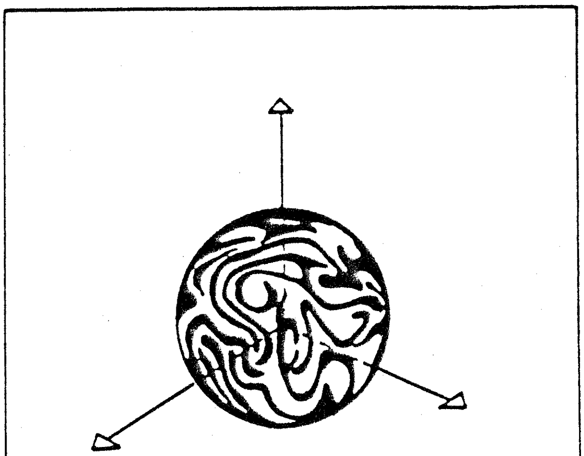

Fig. 3. Schematic illustration of fine structures developed on a constant energy surface.

The fine structures are localized in certain fine structure regions whose linear dimensions are considerably larger than the fine structures therin[7]. These regions appear in the highly stanied 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

$$\gamma^* = (\frac{u^*}{u'})^3 \qquad (18)$$

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

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

giving the following expression

$$\gamma_\lambda = \frac{u^*}{u'} \qquad (20)$$

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

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

and

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

Similarly by introducing the turbulence Reynolds number

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

and

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

Kuo and Corrsin[6] have given some results for the flatnes 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 flatnes factor and the intermittency factor:

$$F_M = 1.5 \cdot (1 + 1/\gamma) \qquad (25)$$

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

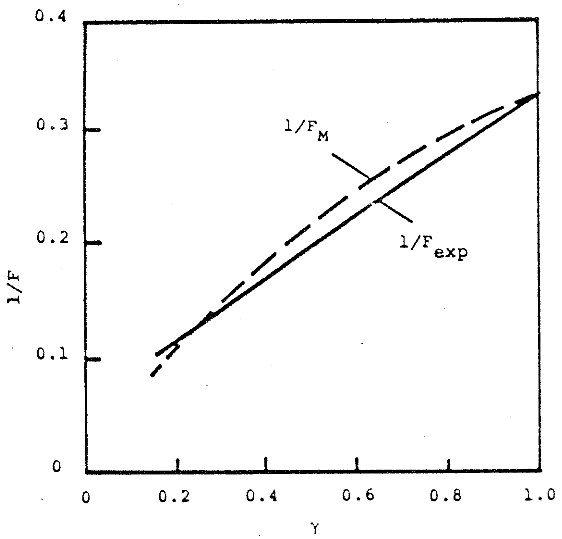

Fig. 4. Comparison between experimental results[10] and empirical expression for the flatnes factor as a function of the intermittency factor.

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

$$F_\lambda = 1.5 + 0.44 \cdot Re_\lambda^{0.5} \qquad (26)$$

Equation (26) is compared with the experimental results of Kuo and Corrsin[6] in fig. 5.

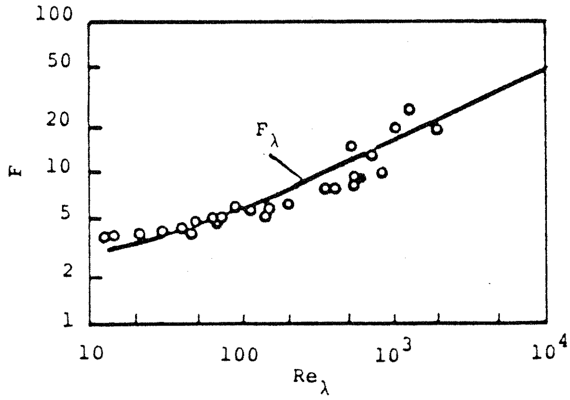

Fig. 5. Flatnes factor of $\partial u/\partial t$ as a function of Re_λ compared with theoretical flatnes factor for the fine structures.

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.

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

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

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

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:

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

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

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

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:

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

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:

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

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 stochiometric 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:

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

where $\bar{c}_{pr}$ is the local mean consentration 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:

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

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

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

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:

$$T^* = \bar{T} + \Delta T \quad (36)$$

and the surrounding temperature:

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

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

Chemical controlled reaction rate

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

The bulk mixing time scale

$$\tau_M = 1/\dot{m} \quad (38)$$

The fine structure time scales

$$\tau^* = \gamma^*/\dot{m} \quad (39)$$

$$\tau_\lambda = \gamma_\lambda/\dot{m} \quad (40)$$

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 to establish criteria for extinction of flames.

Some results

The following shows some few calculation results.

Figure 6 shows a comparison between calculation[11] and experimental data[12] for a hydrogen diffusion flame.

Figure 7 similarly shows a comparison between experimental and calculated soot concentrations for turbulent diffusion flames [1].

Figure 8 compares experimental and calculated oxygen concentrations in a premixed flame. These calculations were performed by a somewhat simplified version of the combustion model[13].

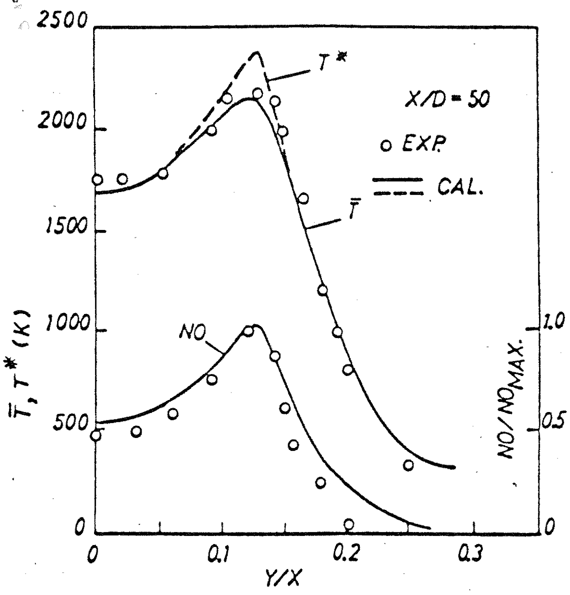

Fig. 6. Radial variation of temperature and nitrogen oxide in a hydrogen diffusion flame.

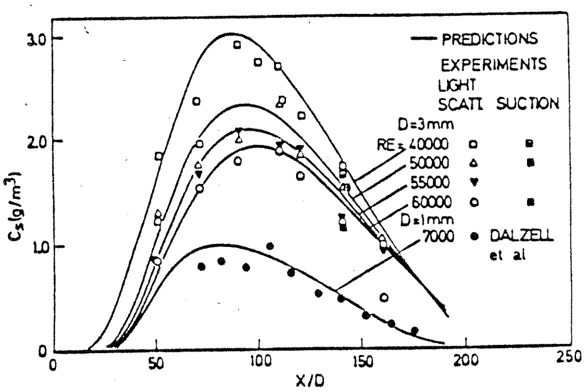

Fig. 7. Experimental and predicted soot consentrations in turbulent diffusion flames.

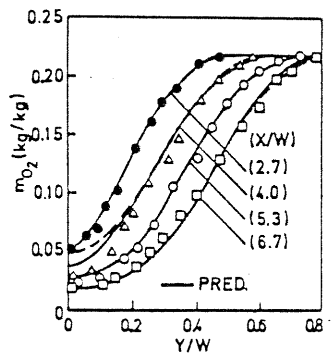

Fig. 8. Experimental and predicted oxygen consentrations in a premixed flame.

Conclusions

The models presented here can readily handle complex chemistry and at the same time take care of turbulence interaction. Results obtained with these models are in close agreement with experimental data.

References

1. Magnussen, B. F., Hjertager, B.H., Olsen, J.G., and Bhaduri, D.: Seventeenth Symposium (International) on Combustion, p. 1383, The Combustion Institute, (1979)
2. Magnussen, B.F.: Fifteenth Symposium (International) on Combustion, p. 1415, The Combustion Institute, (1975)
3. Kolmogorov, A.N.: J. Fluid Mech., 13, 82, (1962)
4. Corrsin, S.: Phys. Fluids, 5, 1301 (1962)
5. Tennekes, H.: Phys. Fluids, 11, 669, (1968)
6. Kuo, A.Y., and Corrsin, S.: J. Fluid Mech., 50, 285, (1971)
7. Kuo, A.Y.: and Corrsin, S.: J. Fluid Mech., 56, 477, (1972)
8. Magnussen, B.F.: Some Features of the Structure of a Mathematical Model of Shear Flow Turbulence, Report, NTH, (1975)
9. Batchelor, G.K., and Townsend, A.A.: Proc. Roy. Soc., A 199, 238, (1949)
10. Wygnanski, I., and Fiedler, H.: J. Fluid Mech., 38, (1969)
11. Magnussen, B.F.: Gen. Mot. Symposium on Part. Carbon Formation During Combustion, (1980)
12. Takagi, T., Ogasawara, M., Fuju, K.,and Daizo, M.: Fifteenth Symposium (International) on Combustion, 1051, The Combustion Institute, (1974)
13. Magnussen, B.F., and Hjertager, B.H.: Sixteenth Symposium (International) on Combustion, p. 719, The Combustion Institute, (1976)