Modeling of NOx and Soot Formation by the Eddy Dissipation Concept

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MODELING OF
POLLUTANT FORMATION IN GAS TURBINE COMBUSTORS BASED ON THE EDDY DISSIPATION CONCEPT.

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ABSTRACT

The Eddy Dissipation Concept (EDC) of Magnussen is a general concept for treating the interaction between the turbulence and the chemistry in flames. It is a reactor concept which identifies a reactor related to the fine structures in turbulence. This reactor is treated as a homogeneous reactor exchanging mass and energy with the surrounding fluid, thus allowing a complete treatment of the chemistry for the reactor.

There are several important technological processes that require inclusion of chemical kinetics. Examples are: pollution formation in burners and engines, knocking in engines, and stabilization of turbulent flames close to extinction. At present a few chemically controlled combustion processes have been calculated by the EDC: soot formation and combustion, NO_x formation, and extinction leading to the lift-off of turbulent jet diffusion flames.

The present paper gives a detailed review of the EDC, and demonstrates the application of the concept with special emphasis on soot and NO_x. The results obtained are in close agreement to experimental data. The paper also discusses the application of the EDC for gas turbine combustors.

INTRODUCTION

The Eddy Dissipation Concept (EDC) of Magnussen has been applied without the need for changing any constants for a great variety of cases where the chemical kinetics is much faster than the turbulence fine structure mixing, by assuming infinite fast chemistry. Such cases have been premixed and diffusion flames, transient development of fires, flares, gas explosions, combustion in Otto engines and gas turbine combustors. Some examples are given in [1-12]. The EDC is also included in the commercially available computer code FLUENT.

The Eddy Dissipation Concept is a general concept for treating the interaction between the turbulence and the chemistry in flames which on one side offers the opportunity to treat the turbulence-chemical kinetic interaction in a stringent conceptional way at the same time as it takes care of many of the important characteristics of turbulence. Important combustion cases were the chemical kinetics have dominating influence on the combustion evolution, like extinction and pollutant formation have been analyzed with promising results, [1,3,4,13].

The following gives a detailed review of the EDC from a principle and practical point og view, and demonstrates and discusses the applicability of this concept for calculation of the combustion in gas turbine combustors with special emphasis on pollutant formation and stability in the combustor.

PRINCIPLE AND PRACTICAL ASPECTS OF THE EDC

The reaction space

Chemical reactions take place when reactants are mixed at molecular scale at sufficiently high temperature [2]. 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 only 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 [14-18].

The fine structures are responsible for the dissipation of turbulence energy 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, as well as for homogeneously mixed reactants in turbulent flow. Such non-homogenity of the reaction space have been demonstrated in a number of recent laser-sheet fluorescense measurements [19].

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 fraction 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 includes basic features of the preceeding.

Turbulence energy dissipation

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

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 through the interstructural straining actions 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 turbulence 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 turbulence length, L´. These quantities are linked to each other through the turbulent eddy viscosity:

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

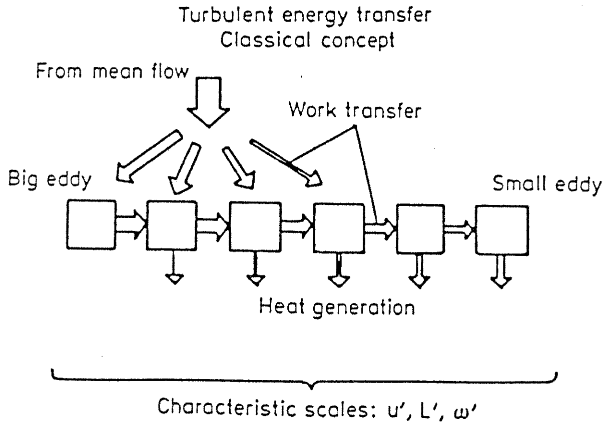


Fig.1. Turbulence energy transfer.

Modelling interstructural energy transfer

Figure 2 schematically illustrates a model for the transfer of mechanical energy from bigger to smaller turbulence structures [20].

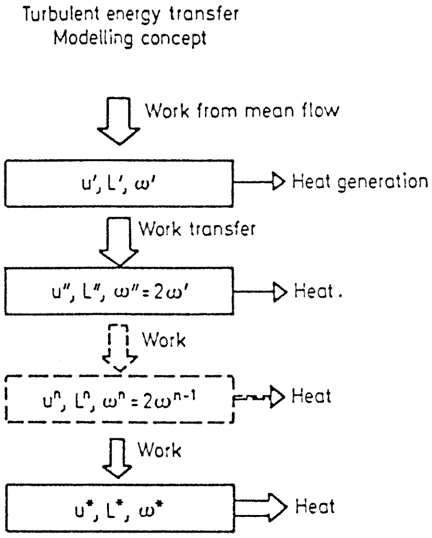


Fig.2. A modelling concept for transfer of energy form bigger to smaller turbulence structures.

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

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

This vorticity is according to the EDC [20] an isotropic quantity

$$\omega' = \frac{u'_1}{L'_1} = \frac{u'_2}{L'_2} = \frac{u'_3}{L'_3} \tag{3}$$

For nearly isotropic turbulence the rate of dissipation can for this level be expressed as

$$\varepsilon' = \xi^2 (12 \frac{u'}{L'} \cdot u''^2 + 15 \cdot \nu (\frac{u'}{L'})^2) \tag{4}$$

where ξ is a numerical constant.

The first term in the bracket of eq. (4) represents the mechanical energy transfer to the next turbulence level while the last term represents the viscous dissipation into heat at the first level.

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

$$\omega'' = 2\omega' \qquad (5)$$

velocity, u'', and length scale, L''.

The turbulence energy balance for the second structure level is consequently given by

$$\xi^2 \, 12 \frac{u'}{L'} u''^2 = \xi^2 \left(12 \frac{u''}{L''} \cdot u'''^2 + 15 \cdot \nu \left(\frac{u''}{L''} \right)^2 \right) \qquad (6)$$

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 structures is expressed by

$$\omega^* = \xi^2 \cdot 6 \frac{u^*}{L^*} \cdot u^{*2} \qquad (7)$$

and the dissipation by

$$q^* = \xi^2 \cdot 15 \nu \left(\frac{u^*}{L^*} \right)^2 \qquad (8)$$

According to this model only a small fraction of the dissipation of energy into heat takes place at the highest level. Similarly it can be shown that approximately 3/4 of the dissipation takes place at the fine strucure level.

The fraction of the dissipation taking place at the highest structural level depends on the turbulence Reynolds number.

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

$$\varepsilon = 0.2 \frac{u'^3}{L'} \qquad (9)$$

$$\varepsilon = 0.267 \frac{u^{*3}}{L^*} \tag{10}$$

$$\varepsilon = 0.67 \, \nu \, (\frac{u^*}{L^*})^2 \tag{11}$$

By combination of eqs. (10) and (11) the following characteristic scales for the fine structures are obtained

$$u^* = 1.74 \, (\varepsilon \cdot \nu)^{1/4} \tag{12}$$

and

$$L^* = 1.43 \, \nu^{3/4}/\varepsilon^{1/4} \tag{13}$$

where u^* is the mass average fine structure velocity, and L^* the characteristic length scale. 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, 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).

The fine structures are localized in certain fine structure regions whose linear dimensions are considerably larger than the fine structures therein [18]. These regions appear in the highly strained regions between the bigger eddies.

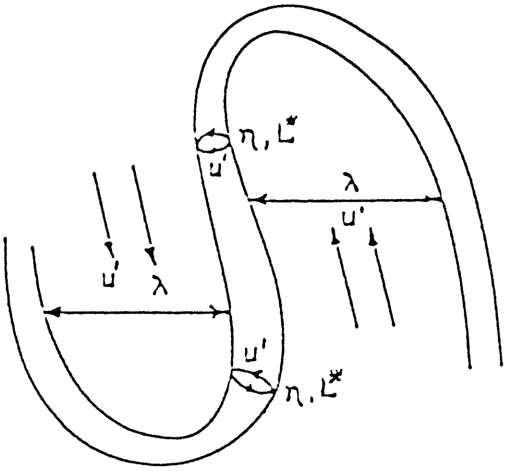


Fig.3. Schematic illustration of fine structure vortex [16].

Modeling 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. 9 and 10) can be expressed by

$$\gamma^* = \left(\frac{u^*}{u'}\right)^3 \qquad (14)$$

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

$$\gamma_\lambda = \frac{u^*}{u'} \qquad (15)$$

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

$$\gamma^* = 9.7 \cdot \left(\frac{\nu\cdot\varepsilon}{k^2}\right)^{\overset{3/4}{\cancel{1/3}}} \qquad (16)$$

and

$$\gamma_\lambda = 2.13 \cdot \left(\frac{\nu\cdot\varepsilon}{k^2}\right)^{1/4} \qquad (17)$$

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 fluid can be expressed as follows

$$\dot{m} = 2 \cdot \frac{u^*}{L^*} \cdot \gamma^* \quad (1/s) \tag{18}$$

Expressed by k and ε for nearly isotorpic turbulence eq.(18) turns into

$$\dot{m} = 23.6 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2}\right)^{1/4} \cdot \frac{\varepsilon}{k} \quad (1/s) \tag{19}$$

or

$$\dot{m} = 11.08 \cdot \gamma_\lambda \cdot \frac{\varepsilon}{k} \quad (1/s) \tag{20}$$

The mass flow per unit of mass of the fine structures may consequently be expressed as

$$\dot{m}^* = 2 \cdot \frac{u^*}{L^*} \quad (1/s) \tag{21}$$

or expressed in terms ε and ν as

$$\dot{m}^* = 2.43(\varepsilon/\nu)^{1/2} \quad (1/s) \tag{22}$$

A fine structure residence time may also be expressed as

$$\tau^* = \frac{1}{\dot{m}^*} \quad (s) \tag{23}$$

Modeling the molecular mixing processes

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

The various species are assumed to be homogeneously mixed within the fine structures.

The mean net mass transfer rate, $\bar{R}_i$, between a certain fraction, χ, of the fine structures and the rest of the fluid, can for a certain specie, i, be expressed as follows:

$$\bar{R}_i = \bar{\varrho} \cdot \dot{m} \cdot \chi \left(\frac{c_i^0}{\varrho^0} - \frac{c_i^*}{\varrho^*} \right) \quad (kg/m^3/s) \tag{24}$$

where * and ^{0} refer to conditions in the fine structures and the surrounding.

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

$$R_i^* = \varrho^* \cdot \dot{m}^* \left(\frac{c_i^0}{\varrho^0} - \frac{c_i^*}{\varrho^*} \right) \quad (kg/m^3/s) \tag{25}$$

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:

$$\frac{\bar{c}_i}{\bar{\varrho}} = \frac{c_i^*}{\varrho^*} \cdot \gamma^* \cdot \chi + \frac{c_i^0}{\varrho^0} \cdot (1 - \gamma^* \cdot \chi) \tag{26}$$

By substitution from eq. (26) into eq. (24) one can express the mass transfer rate between a certain fraction, χ, of the fine structures and the surrounding fluid as

$$\bar{R}_i = \frac{\bar{\varrho} \cdot \dot{m} \cdot \chi}{1 - \gamma^* \cdot \chi} \left(\frac{\bar{c}_i}{\bar{\varrho}} - \frac{c_i^*}{\varrho^*} \right) \quad (kg/m^3/s) \tag{27}$$

and consequently per unit volume in the fine structure fraction, χ, as

$$R_i^* = \frac{\varrho^* \cdot \dot{m}^*}{1 - \gamma^* \cdot \chi} \left(\frac{\bar{c}_i}{\bar{\varrho}} - \frac{c_i^*}{\varrho^*} \right) \quad (kg/m^3/s) \tag{28}$$

Modelling the reaction processes

The net mean transfer rate of a certain specie, i, from the surrounding fluid into the fine structures equals the mean consumption rate of the same specie within the fine structures.

If the reactions are assumed to take place within the fine structures, the reaction can be described as in the following figure:

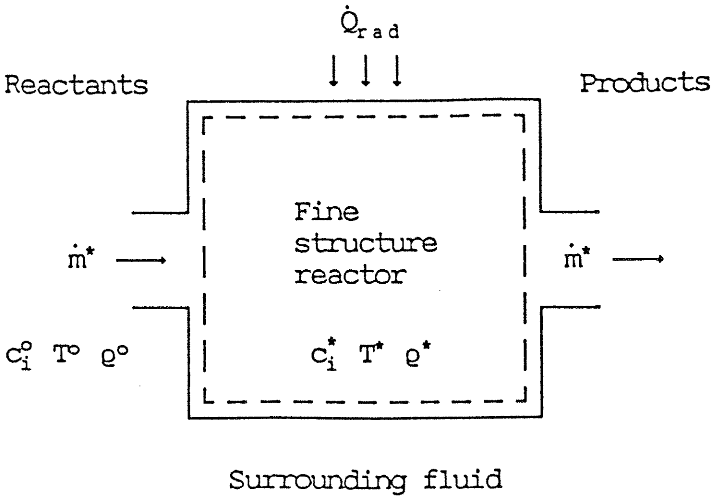


Fig. 4. Schematic illustration of a reacting fine structure.

On the basis of the assumption of the fine structure reactor being homogenously mixed, the net consumption rate of a specie, i, is determined by the reaction rate, taking into consideration all relevant species and their chemical interaction and the local conditions within the reactor. Thus in addition to solving the necessary equations for the chemistry one has to solve an additional equation for the energy balance as follows:

$$q^* = \frac{\varrho^* \cdot \dot{m}^*}{1-\gamma^* \cdot \chi} \cdot \sum_i^N \left(\frac{\bar{c}_i}{\bar{\varrho}} \cdot \bar{h}_i - \frac{c_i^*}{\varrho^*} \cdot h_i^* \right) \tag{29}$$

where, $\bar{h}_i$, and, h_i^*, are the total enthalpies for each specie, and q^* the net energy being stored in the reacting fine structures or transferred from the fine structures to the surroundings by other mechanisms like radiation.

When treating reactions, χ designates the reacting fraction of the fine structures. Only the fraction, χ, which are sufficiently heated will react.

The fraction of the fine structures which may react can be assumed proportional to the ratio between the local concentration of reacted fuel and the total quantity of fuel that might react:

$$\chi = \frac{1}{\gamma_\lambda} \frac{\bar{c}_{pr}/(1+r_{fu})}{\bar{c}_{pr}/(1+r_{fu}) + \bar{c}_{min}} \cdot R_{ij} \tag{30}$$

where, $\bar{c}_{pr}$ is the local mean concentration of reaction products, $\bar{c}_{min}$ the smallest of $\bar{c}_{fu}$ and $\bar{c}_{O_2}/r_{fu}$, and r_{fu} the stochiometric oxygen requirement, and R_{ij} a correlation factor for nonpremixedness of reactants.

The appearance of γ_λ in eq.(30) implies the assumption that the reaction products, which are formed within the fine structure regions, may have a higher concentration within these regions than the mass average concentrations, and thus increase the probability of ignition of non-reacted fine structures according to eq. (30).

From physical and conceptional reasons χ must be limited according to

$$\chi \leq R_{ij} \tag{31}$$

In a simplified form R_{ij} may be expressed as follows:

$$R_{ij} = \frac{(\bar{c}_{min} + c_{Pr}/(1+r_{fu}))^2}{(\bar{c}_{fu} + \bar{c}_{pr}/(1+r_{fu}))(\bar{c}_{O_2}/r_{fu} + \bar{c}_{pr}/(1+r_{fu}))} \tag{32}$$

For stochiometric premixed flames, R_{ij} equals unity.

A detailed analysis of computational results for the flame propagation in premixed gases have indicated that the combination of eqs. (27), (28), (29), (30), (31) and (32) tends to give too low reaction rates in the tale of the flame. This can be explained physically as follows:

The time mean, mass average concentrations of reactants will be low in these regions, however, the concentrations of the reactants in the non-reacted structures which are separated from the reacted structures by thin reacting interfaces will still be high. The reacting fine structures will consequently catch up reactants at a higher rate than predicted by eqs. (27) and (28).

If it is assumed that the non-reacted fluids in the ~~tale~~ tail of the flame have been entrained into the fine structure regions, one may introduce a parameter, η, such that

$$\bar{R}_i = \eta \cdot \bar{R}_i \text{ (eq.27)} \tag{33}$$

and

$$R^*_i = \eta \cdot R^*_i \text{ (eq. 28)} \tag{34}$$

where η is expressed as

$$\eta = \frac{1}{\gamma_\lambda} \tag{35}$$

with the following limitation

$$\eta \cdot \frac{\bar{c}_{min}}{\bar{c}_{pr}/(1+r_{fu})+\bar{c}_{min}} \leq 1 \qquad (36)$$

consequently

$$\eta \leq \frac{\bar{c}_{pr}/(1+r_{fu})+\bar{c}_{min}}{\bar{c}_{min}} \qquad (37)$$

Including the preceeding the expressions for the reaction rates, eq. (27) and eq. (28) can now be expressed as follows:

$$\bar{R}_i = \frac{\bar{\varrho}\cdot\dot{m}\cdot\chi\cdot\eta}{1-\gamma^*\cdot\chi}\left(\frac{\bar{c}_i}{\bar{\varrho}} - \frac{c_i^*}{\varrho^*}\right) \quad (\mathrm{kg/m^3/s}) \qquad (38)$$

$$R_i^* = \frac{\varrho^*\cdot\dot{m}^*\cdot\eta}{1-\gamma^*\cdot\chi}\left(\frac{c_i}{\bar{\varrho}} - \frac{c_i^*}{\varrho^*}\right) \quad (\mathrm{kg/m^3/s}) \qquad (39)$$

The equation for the energy balance of the reacting fine structures, eq. (29) transforms into:

$$q^* = \frac{\varrho^*\cdot\dot{m}\cdot\eta}{1-\gamma^*\cdot\chi}\cdot\sum_i^N\left(\frac{\bar{c}_i}{\bar{\varrho}}\cdot\bar{h}_i - \frac{c_i^*}{\varrho^*}\cdot h_i^*\right) \quad (\mathrm{kg/m^3/s}) \qquad (40)$$

According to the EDC the preceeding gives the necessary quantitative format for full chemical kinetic treatment of the reacting fine structures in turbulent premixed and diffusion flames. The method can readily be extended to treatment of reactions also in the surrounding fluid, which may be necessary for the treatment of for instance NO_x formation in premixed flames.

The mean reaction rate can in this case be expressed as

$$\frac{\bar{R}_i}{\bar{\varrho}} = \gamma^*\cdot\chi\,\frac{R_i^*}{\varrho^*} + (1-\gamma^*\cdot\chi)\frac{R_i^0}{\varrho^0} \qquad (41)$$

where R_i^0 is the reaction rate in the surrounding fluid.

The fast chemistry limit.

In a great number of combustion cases, the infinite fast chemistry limit treatment of the reactions is sufficient. In this case eqs. (38) and (39) transforms into

$$\bar{R}_{fu} = \frac{\bar{\varrho}\cdot\dot{m}\cdot\chi\cdot\eta}{1-\gamma^{*}\cdot\chi}\cdot\bar{c}_{min}\frac{1}{\xi} \quad (kg/m^3/s) \qquad (42)$$

$$R^{*}_{fu} = \frac{\varrho^{*}\cdot\dot{m}^{*}\cdot\eta}{1-\gamma^{*}\cdot\chi}\cdot\bar{c}_{min}\frac{1}{\xi} \quad (kg/m^3/s) \qquad (43)$$

The temperature of the reacting fine structures and the surrounding fluid may be expressed as

$$T^{*} = \bar{T} + \frac{\bar{c}_{min}\cdot\Delta H_R}{\bar{\varrho}\cdot c_p} - \frac{q^{*}(1-\gamma^{*}\cdot\chi)}{\varrho^{*}\cdot c_p\cdot\dot{m}^{*}\cdot\eta} \qquad (44)$$

and

$$T^{0} = \bar{T} - \frac{\bar{c}_{min}\cdot\Delta H_R}{\bar{\varrho}\cdot c_p}\cdot\frac{\gamma^{*}\cdot\chi}{1-\gamma^{*}\cdot\chi} + \frac{q^{*}\cdot\gamma^{*}\cdot\chi}{\varrho^{*}\cdot c_p\cdot\dot{m}^{*}\cdot\eta} \qquad (45)$$

where, ΔH_R is the heat of reaction (kJ/kg fuel), and c_p the local specific heat (kJ/kg/K).

The reaction rate expressed by eq. (42) implies a turbulent flame propagation velocity in premixed gases [4]:

$$U_B \approx 2\left(\frac{\dot{m}\cdot\nu_t}{\gamma_\lambda\cdot\sigma_{fu}}\right)^{1/2} \qquad (46)$$

where, ν_t is the turbulence viscosity, and σ_{fu} the Prandtl/Schmidt number.

Introduction of the turbulence quantities; k, the turbulence kinetic energy, and ε, its rate of dissipation leads to

$$U_B \approx 2\left(\frac{k}{\sigma_{fu}}\right)^{1/2} \qquad (47)$$

MODELING POLLUTANT FORMATION

Modeling of soot formation and combustion in turbulent flames.

The modeling of soot formation can be based on the two equations as used previously by Magnussen et al. [1,3,5].

An equation for the rate of formation of radical nuclei is expressed by

$$R_{n,f} = n_o + (f-g)n - g_o n N \qquad (\text{part/m}^3/\text{s}) \qquad (48)$$

where, n is the concentration of radical nuclei, N is the concentration of soot particles and n_o is the rate of spontaneous formation of radical nuclei expressed by

$$n_o = 1.08 \cdot a_o \cdot fc \cdot \bar{c}_{fu} \cdot \exp(-E/RT) \quad (\text{part/m}^3/\text{s}) \qquad (49)$$

where $\bar{c}_{fu}$ is the mean concentration of fuel (kg/m³), and fc is the mass fraction of carbon in the fuel.

The rate of soot particle formation is expressed by

$$R_{s,f} = m_p (a - bN)n \qquad (\text{kg/m}^3/\text{s}) \qquad (50)$$

where m_p= is the mass of a soot particle (kg/part).

These equations were first proposed by Tesner et al. [21,22]. Equation (49) has been modified to be applicable to other fuels than acetylene.

The following constants can be applied:

$a=10^5$, $f-g=10^2$, $g_o=10^{-15}$, $b=8\cdot 10^{-14}$, $E/R=9\cdot 10^4$, and $\varrho_s=2(\text{g/cm}^3)$.

The constant, a_o, is dependent on the soot particle diameter as follows:

$$d_p^3 \cdot a_o = \text{constant} \qquad (51)$$

with the value $a_o = 12.5\cdot 10^{36}$ part/kg/s for $d_p=178.5$ A (Angstrom) [1,3].

If soot is allowed to be formed both in the heated fine structures and in the surrounding fluid, and it is assumed that the mass fraction of the fuel contained in the heated fine structures is proportional to $\gamma^* \cdot \chi$, local equilibrium with the surrounding fluid for the fine structures leads to the following equations:

$$R^*_{n,f} - \frac{\bar{\varrho}\cdot\dot{m}^*\cdot\eta}{1-\gamma^*\cdot\chi}\left(\frac{n^*}{\varrho^*} - \frac{\bar{n}}{\bar{\varrho}}\right) = 0 \qquad (52)$$

and

$$R^*_{s,f} - \frac{\bar{\varrho}\cdot\dot{m}^*\cdot\eta}{1-\gamma^*\cdot\chi}\left(\frac{c^*_s}{\varrho^*} - \frac{\bar{c}_s}{\bar{\varrho}}\right) = 0 \qquad (53)$$

The mean rates of formation can then be expressed by

$$\bar{R}_{n,f} = n_{o,T^*}\gamma^*\chi\bar{\varrho}/\varrho^* + n_{o,T^0}(1-\gamma^*\chi)\bar{\varrho}/\varrho^0 \qquad (54)$$

$$+(f-g)\bar{n} - g_0 n^* N^* \gamma^* \chi\bar{\varrho}/\varrho^* - g_0 n^0 N^0 (1-\gamma^*\chi)\bar{\varrho}/\varrho^0$$

and

$$\bar{R}_{s,f} = m_p(a-bN^*)n^*\gamma^*\chi\bar{\varrho}/\varrho^* + m_p(a-bN^0)n^0(1-\gamma^*\chi)\bar{\varrho}/\varrho^0 \qquad (55)$$

The mean rates of nucleus and soot particle combustion can be as follows:

$$\bar{R}_{n,c} = \bar{R}_{fu}\bar{n}/\bar{c}_{fu} \qquad (\mathrm{part/m^3/s}) \qquad (56)$$

and

$$\bar{R}_{s,c} = \bar{R}_{fu}\bar{c}_s/\bar{c}_{fu} \qquad (\mathrm{kg/m^3/s}) \qquad (57)$$

The following figure gives an example of computational results in comparison with experimental data. [5]

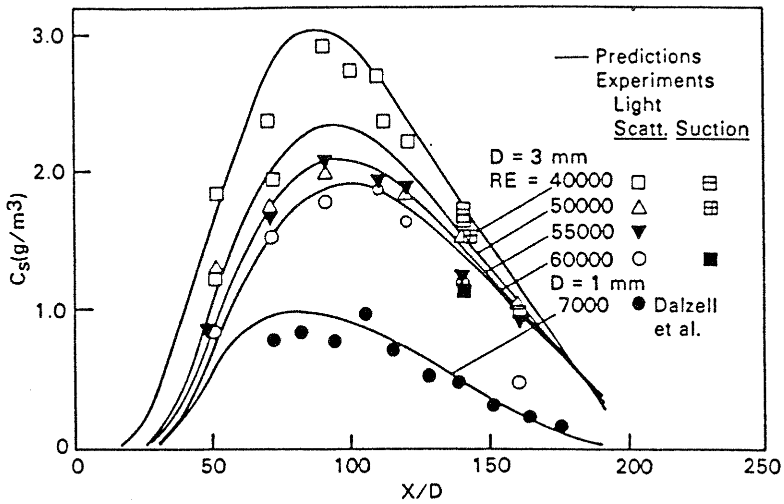


Fig. 5. Variation of mean value of soot concentration along the axis of acetylene diffusion flames. Comparison between prediction and experimental results.

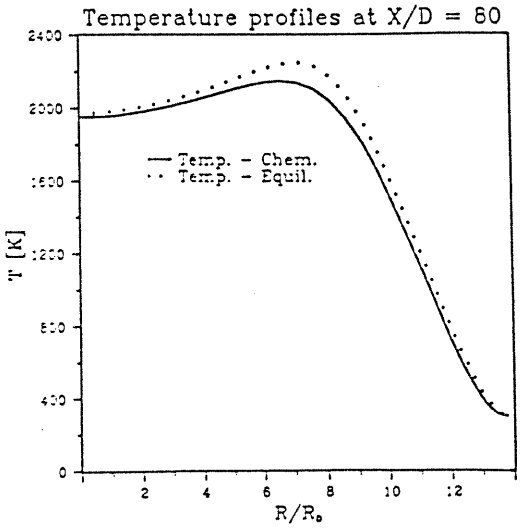
This model has been used for a variety of fuels under different combustion conditions with very reasonable results.

Modeling of NO_x formation in a turbulent diffusion flame.

The following presents some results [13] of a chemical treatment of the fine structures in two alternatives; chemical equilibrium and full chemistry for a hydrogen-air jet diffusion flame. The reactions in the surrounding fluid have been considered frozen.

For the chemical equilibrium calculations the STANJAN code of Reynolds in connection with the CHEMKIN program library of Kee and Miller were used. For the chemical kinetic calculations the PSR code of Kee, Miller and Glarborg was used [21,22].

Figures 6 and 7 show that the mean temperature and main species are just moderately influenced by the chemical kinetics.



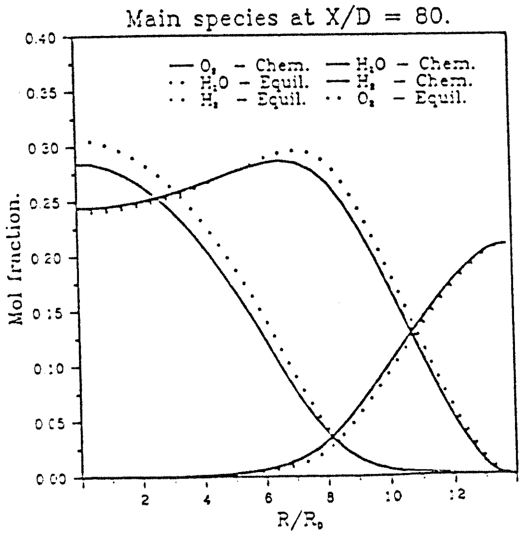


Fig.6. Calculated radial profile of mean temperature.

Fig.7. Calculated radial profile of mean species.

Figure 8 shows a radial profile of NO in which the chemical kinetic effect is demonstrated.

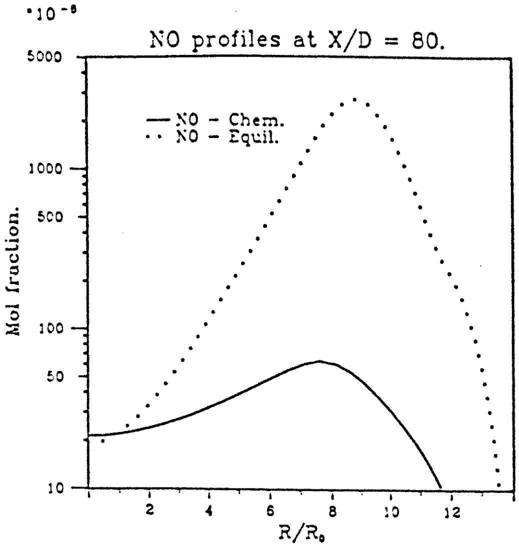


Fig.8. Calculated radial profile of NO.

Figure 9 and 10 demonstrate the same effect on two of the importante intermediate species.

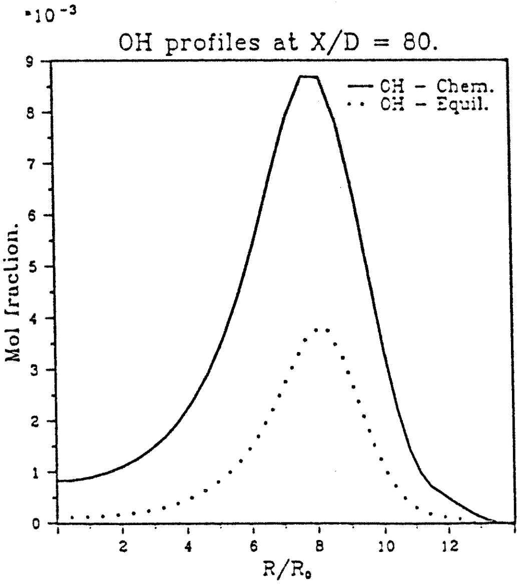


Fig.9. Calculated radial profile of OH.

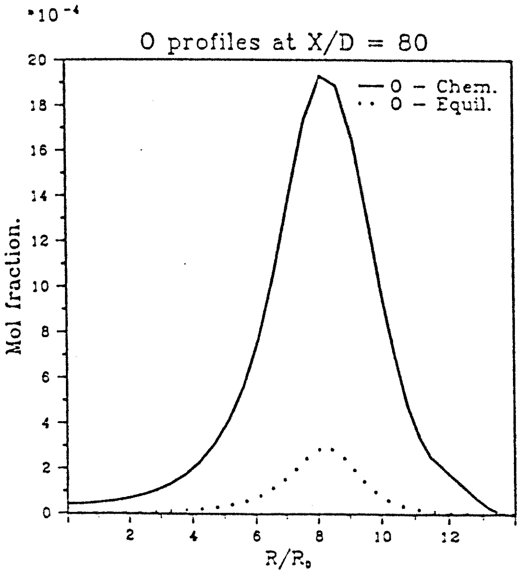


Fig.10. Calculated radial profile of O.

The results demonstrated here are very promising and close to experimental data.

The results also indicate the way in which pollutant formation and destruction can be modeled in complicated environments like the gas turbine combustor viz.:

- First the main species and temperatures including the fine structure temperature are calculated on the basis of an assumption of one step forward reaction or chemical equilibrium in the fine structures, tests must simultaneously be conducted for local extinction effect [4], then the chemistry for the minor species are superimposed, opening for a significant reduction of the chemical kinetic schemes.

- The other alternative is to apply full chemistry according to the method for every point in time and space.

The flame stability may similarly be evaluated either in a simplified way by comparison between a characteristic fine structure time scale [4] or by application of full chemistry.

CONCLUSION

The preceeding have presented the most updated version of the EDC of Magnussen with application to full chemical treatment of pollutant formation and destruction, relevant to gas turbine combustors. It may be concluded that this concept offers the opportunity to include chemistry at various complication levels, in a straight forward way and there is no need for problem dependent adjustments of any constant according to the concept.

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