

# A MODIFIED SOLUTION PROCEDURE FOR THE ELLIPTIC-TYPE CONDITIONAL MOMENT CLOSURE MODEL IN NONPREMIXED TURBULENT REACTING FLOW

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## ABSTRACT

The conditional moment closure formulation considering the molecular and turbulent diffusion is derived. A simplified solution procedure is proposed to reduce the computational burden due to the increased dimensionality of the conditionally averaged variables. A conditionally averaged variable is expressed as a linear weighted average of the two extremes, 'no reaction' and 'equilibrium' states. The modified elliptic-type conditional moment closure formulation is implemented to simulate a two dimensional nonpremixed mixing layer reacting flow. Results show good agreement for the conditional averages of the species concentration in Bilger et al.

## 1. INTRODUCTION

The coupling of instantaneous, turbulent scalar fluctuations with nonlinear Arrhenius kinetical expressions makes it difficult to accurately model and predict the combustion system by the commonly employed unconditional averaging approaches[1,2]. A new closure procedure, named the CMC (Conditional Moment Closure) was proposed by Klimenko and Bilger[3, 4, 5]. This approach does not assume any local physical picture of the reacting flow but predicts averages conditional on the mixture fraction. Although it increases the dimensionality of the problem, it eliminates the major source of nonlinearity resulting from closure for the reaction rate term. This method has the advantage of effectively decoupling chemical kinetics from the large inhomogeneity of a turbulent flow while preserving the input from the scalar dissipation. Arbitrarily complex kinetics may be used to obtain detailed flow and reaction information without substantial increase in computational cost.

In the original CMC formulation there exists limitation for its practical applications. The original CMC equation is derived on the basis of high Reynolds number assumption, which neglects the molecular diffusion effect. The turbulent diffusivity has also been neglected in the previous studies. There may be some numerical difficulties to apply the original CMC formulation to multidimensional elliptic problems because of inconsistency with other governing equations and stiffness of the kinetic system. In the present work, the rederived CMC equation is in a conservative form and retains the molecular and turbulent diffusion terms. A

two-dimensional computing code is developed and applied to a simple nonpremixed turbulent diffusion reacting flow with assumed probability density for the mixture fraction and the  $k-\varepsilon-g$  turbulence model.

A simplified procedure is proposed here to avoid the problem of increased dimensionality due to conditioning on the mixture fraction in the CMC method. It is based on some simplifying assumptions with engineering applications in mind.

## 2. EQUATION DERIVATION

### 2.1 *Elliptic-type formulation*

Consider the conservation equation for the mass fraction of the  $i$ -th species,  $Y_i$ , obeying Fick's law of diffusion with variable physical properties.

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{U} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + w_i \quad (1)$$

The mixture fraction is defined as,

$$\xi = \frac{\beta - \beta_O}{\beta_F - \beta_O} \quad (2)$$

where  $\beta$  is any conserved scalar. The subscripts 'O' and 'F' denote the oxidizer and fuel respectively. The mixture fraction obeys the conservation equation,

$$\frac{\partial}{\partial t}(\rho \xi) + \nabla \cdot (\rho \vec{U} \xi) = \nabla \cdot (\rho D \nabla \xi) \quad (3)$$

with  $D$  the properly chosen mean diffusivity dependent on the definition of  $\beta$ .

For variable property flow, the density weighting, or Favre's averaging, technique is used. There exist following relations,

$$Y_i = Q(\xi) + y \quad (4)$$

$$\vec{U} = \vec{U}_\xi + \vec{u} \quad (5)$$

$$\vec{U}_\xi = \frac{\langle \rho \vec{U} | \xi \rangle}{\langle \rho | \xi \rangle} \quad (6)$$

$$Q(\xi) = \frac{\langle \rho Y_i | \xi \rangle}{\langle \rho | \xi \rangle} \quad (7)$$

$$\rho_\xi = \langle \rho | \xi \rangle \quad (8)$$

where the angular bracket denotes the ensemble average over an ensemble of realizations and the vertical bar indicates that this average is conditional on the condition  $\xi(\vec{x}, t) = \xi$ . The symbols,  $\vec{u}$  and  $y$ , are the fluctuations from the density weighted conditional averages of  $\vec{U}$  and  $Y_i$ .

Following Bilger's derivation procedure[5],

$$\begin{aligned} w(\vec{x}, t) &= \frac{\partial Q}{\partial t} + \rho \vec{U} \cdot \nabla Q - \rho D_i (\nabla \xi \cdot \nabla \xi) \frac{\partial^2 Q}{\partial \xi^2} \\ &- \nabla \cdot [\rho D_i \nabla Q] - \rho D_i \nabla \xi \cdot \nabla \frac{\partial Q}{\partial \xi} - \frac{\partial Q}{\partial \xi} \nabla \cdot [\rho (D_i - D) \nabla \xi] \\ &+ \rho \frac{\partial y}{\partial t} + \rho \vec{U} \cdot \nabla y - \nabla \cdot (\rho D_i \nabla y) \end{aligned} \quad (9)$$

Here the CMC equation will be rederived from Eq.(9) with modeling assumptions listed in the following. By using the continuity equation, the time and advective terms in Eq.(9) can be rewritten as,

$$\rho \frac{\partial Q}{\partial t} + \rho \vec{U} \cdot \nabla Q = \frac{\partial}{\partial t}(\rho Q) + \nabla \cdot (\rho \vec{U} Q) \quad (10)$$

$$\rho \frac{\partial y}{\partial t} + \rho \vec{U} \cdot \nabla y = \frac{\partial}{\partial t}(\rho y) + \nabla \cdot (\rho \vec{U} y) \quad (11)$$

It is assumed that  $\partial(\rho D_i)/\partial \xi = 0$  and  $\partial[\rho(D_i - D)]/\partial \xi = 0$  since the product of the density and diffusivity is nearly constant as a rough approximation. According to this assumption the third and the sixth term on the right hand side of Eq.(9) can be changed as,

$$\rho D_i (\nabla \xi \cdot \nabla \xi) \frac{\partial^2 Q}{\partial \xi^2} = \frac{\partial}{\partial \xi} [\rho D_i (\nabla \xi \cdot \nabla \xi) \frac{\partial Q}{\partial \xi}] \quad (12)$$

$$\frac{\partial Q}{\partial \xi} \nabla \cdot [\rho (D_i - D) \nabla \xi] = \frac{\partial}{\partial \xi} \{ \nabla \cdot [\rho (D_i - D) \nabla \xi] Q \} \quad (13)$$

Then Eq.(9) becomes,

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho Q) + \nabla \cdot (\rho \vec{U} Q) + \frac{\partial}{\partial \xi} \{ \nabla \cdot [\rho (D - D_i) \nabla \xi] Q \} \\ & = \nabla \cdot \rho D_i \nabla Q + \frac{\partial}{\partial \xi} [\rho D_i (\nabla \xi \cdot \nabla \xi) \frac{\partial Q}{\partial \xi}] + \rho D_i \nabla \xi \cdot \nabla \frac{\partial Q}{\partial \xi} \\ & - \frac{\partial}{\partial t}(\rho y) - \nabla \cdot (\rho \vec{U} y) + \nabla \cdot (\rho D_i \nabla y) + w \end{aligned} \quad (14)$$

Equation (14) is in a conservative form. Taking the expectation of Eq.(14) conditional on  $\xi(\vec{x}, t) = \eta$ , and using Eqs.(4) ~ (8) yields,

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho_\eta Q) + \nabla \cdot (\rho_\eta \langle \vec{U} | \eta \rangle Q) + \frac{\partial}{\partial \eta} \{ \nabla \cdot [\rho_\eta (D - D_i) \langle \nabla \xi | \eta \rangle] Q \} \\ & = \nabla \cdot (\rho_\eta D_i \nabla Q) + \frac{\partial}{\partial \eta} (\rho_\eta D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle \frac{\partial Q}{\partial \eta}) - \nabla \cdot \langle \rho \vec{u} y | \eta \rangle \\ & + \rho_\eta D_i \langle \nabla \xi | \eta \rangle \cdot \nabla \frac{\partial Q}{\partial \eta} + \langle \nabla \cdot (\rho D_i \nabla y) | \eta \rangle + \langle w | \eta \rangle \end{aligned} \quad (15)$$

where  $Q$  is now a function of the nonrandom variable  $\eta$ , instead of the random variable  $\xi$ . The molecular diffusion terms of  $y$  and  $\xi$  are ignored as negligible in comparison with the corresponding turbulent diffusion terms,

$$\nabla \cdot [\rho_\eta (D - D_i) \langle \nabla \xi | \eta \rangle] \approx 0$$

$$\nabla \cdot (\rho_\eta D_i \langle \nabla y | \eta \rangle) \approx 0$$

By assuming  $\nabla(\partial Q/\partial \eta) \approx 0$ , we have,

$$\rho_\eta D_i \langle \nabla \xi | \eta \rangle \cdot \nabla \frac{\partial Q}{\partial \eta} \approx 0$$

This implies that the gradient of  $Q$  with respect to  $\eta$  is approximately constant throughout the spatial domain. It is based on the measurement results in the transverse direction of the mixing layer[6] and the calculation results along the axis downstream of a jet flow[7].

Although the turbulent fluctuation term,  $\nabla \cdot \langle \rho \vec{u} y | \eta \rangle$ , has been argued not to be of the first order in some simple flows[5], the eddy viscosity concept is employed with engineering applications in mind in this paper. It has been considered acceptable in many practical simulations without any conclusive evidence against it yet. The term including  $D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle$  is the conditional scalar dissipation rate to account for the diffusion effect in the  $\eta$  direction. The average scalar dissipation rate may be related to the mean turbulence parameters such as the turbulent kinetic energy, the turbulent kinetic energy dissipation rate, the mean mixture fraction and its variance and the appropriately chosen probability density function[8]. The final form of the rederived CMC equation is now,

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho_\eta Q) + \nabla \cdot (\rho_\eta \vec{U}_\eta Q) \\ & = \nabla \cdot (\rho_\eta D_i \nabla Q - \langle \rho \vec{u} y | \eta \rangle) + \frac{\partial}{\partial \eta}(\rho_\eta D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle \frac{\partial Q}{\partial \eta}) + \langle w | \eta \rangle \end{aligned} \quad (16)$$

Equation (16) is in a conservative form suitable for general elliptic multi-dimensional problems. It is flexible for implementation in different solution algorithms, whether implicit or explicit.

## 2.2 Simplified approach

Since the conditional average of the  $i$ -th species concentration,  $Q$ , is a function of  $t$ ,  $\vec{x}$  and  $\eta$ , its numerical solution involves a significant computational load due to discretization in each coordinate direction. A simplified procedure is proposed here by assuming the functional relationship that,

$$Q(t, \vec{x}, \eta) = (1 - \zeta) Q_{nr}(\eta) + \zeta Q_{eq}(\eta) \quad (17)$$

where  $\zeta = \zeta(t, \vec{x})$ . The variable  $\zeta$  is the reaction progress variable between 'no reaction' and 'equilibrium' states which respectively correspond to  $\zeta=0$  and  $\zeta=1$  as shown in Fig. 1. The profile of  $Q$  with respect to  $\eta$  is assumed to be that from linear interpolation between the two extreme states. The fast chemistry limit simply corresponds to the case of  $\zeta=1$  throughout the domain. By inserting Eq.(17) into Eq.(16) we get,

$$\begin{aligned} & [Q_{eq}(\eta) - Q_{nr}(\eta)] \left\{ \frac{\partial}{\partial t}(\rho_\eta \zeta) + \nabla \cdot (\rho_\eta \vec{U}_\eta \zeta) - \nabla \cdot \rho_\eta D_i \nabla \zeta \right\} \\ & = \langle w | \eta \rangle + \frac{\rho_\eta \chi}{2} \left[ \zeta \frac{\partial^2 Q_{eq}}{\partial \eta^2} + (1 - \zeta) \frac{\partial^2 Q_{nr}}{\partial \eta^2} \right] \end{aligned} \quad (18)$$

To obtain a solution for Eq.(18) the mixture fraction  $\eta$  may be put equal to the local average value at the given timing and location. The variables  $\rho_\eta$  and  $\vec{U}_\eta$  may also be given the local average values without the suffix  $\eta$ . It is shown in Fig.1 that  $Q_{nr}$  varies linearly with  $\eta$  so that its second derivative is equal to zero. The second derivative of  $Q_{eq}$  with respect to  $\eta$  may also be neglected for further simplification since it only has the effect of smoothing the profile of  $Q$  near the

stoichiometric  $\eta$ .

The approach here may be easily adapted to a general computational fluid dynamic solution procedure. The transport equations for the average and fluctuation of the mixture fraction are usually solved in connection with the mass, momentum and energy conservation equations. The above Eq.(18) for the reaction progress variable,  $\zeta$ , may be solved simultaneously with the other transport equations. Care needs to be taken to avoid a null solution for  $\zeta$  at  $\eta=0$  and  $\eta=1$  in Eq.(18). For one step irreversible nonpremixed reacting flow, the equilibrium and the frozen limit values are simply the function of the local mixture fraction and can be readily obtained. Note that all the scalar variables such as the temperature and the species concentration may be given in terms of  $\eta$  and  $\zeta$  as the weighted average by the assumed probability density function for  $\eta$ . Once we get the solution for  $\zeta$ , it may be inserted into Eq.(17) to get the conditional average,  $Q$ .

The simplified approach here is more realistic than the concept of Imperfectly Stirred Reactor(ISR)[9] in the sense that it may consider both the temporal and the spatial variation of the conditional average  $Q$ . The ISR assumes homogeneous  $Q$  with no variation in space, which may only be valid in a strongly recirculating well-mixed device. Implementation of the simplified approach introduced here is now under way and the results will be reported later.

To consider the fluctuation in  $\zeta$  the doubly conditional moment closure formulation should be employed instead of the singly conditional moment closure, Eq.(9). It is straightforward to extend Eq.(18) to the doubly conditional moment closure formulation in terms of  $\eta$  and  $\zeta$  if an appropriate transport equation for the fluctuation in  $\zeta$  is taken into account with its effect on the mean reaction rate. The underlying assumption for the singly conditional moment closure is that the effect of turbulence is primarily due to the fluctuation in  $\eta$ , while the fluctuation in  $\zeta$  has a negligible effect on the mean reaction rate.

### 3. MODELING AND CALCULATION OF TWO-DIMENSIONAL TURBULENT MIXING LAYER COMBUSTION

In the present work, the newly derived CMC equation is implemented to simulate the  $NO-O_3$  reaction system for validation and comparison against available experimental data. The working section is 8 m in length with a diameter of 2.8 m separated by a splitter plate to form two streams, which are doped with  $NO$  and  $O_3$  gases respectively[6]. Because of the low inlet reactants concentrations and low reaction heat release, this reaction is taken as passive. The mixing characteristics will not be dependent on the concentrations and whether reaction is occurring or not.

For two-dimensional planar, turbulent and steady state gas flow, the governing equation for the conditional averaged  $Q$  of the species  $Y_i$  is given from Eq.(16) as,

$$\begin{aligned} & \frac{\partial}{\partial x}(\rho \langle U | \eta \rangle Q) + \frac{\partial}{\partial y}(\rho \langle V | \eta \rangle Q) \\ &= \frac{\partial}{\partial x}(\rho D_{t,i} \frac{\partial Q}{\partial x}) + \frac{\partial}{\partial y}(\rho D_{t,i} \frac{\partial Q}{\partial y}) + \frac{\partial}{\partial \eta}[\rho D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle \frac{\partial Q}{\partial \eta}] + \langle w | \eta \rangle \end{aligned} \quad (19)$$

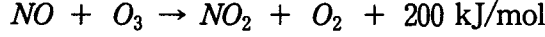
where  $D_{t,i}$  is the turbulent diffusivity which includes the turbulent transport,  $\vec{u} \cdot \nabla$ . The conditional averages of  $\langle U | \eta \rangle$ ,  $\langle V | \eta \rangle$  and  $D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle$  are replaced by the unconditional averages  $U$ ,  $V$  and  $\overline{\nabla \xi \cdot \nabla \xi}$ . Turbulent shear stress is calculated by the  $k-\epsilon$  two equation turbulence model. The mean scalar dissipation  $\bar{\chi}$  is given,

by the equality of velocity and scalar integral length scales, as,

$$\bar{\chi} = D_i \langle \nabla \xi \cdot \nabla \xi | \eta \rangle \approx c_\chi \varepsilon g / k \quad (20)$$

where  $k$  is the mean turbulent kinetic energy,  $\varepsilon$  the turbulent energy dissipation rate,  $g$  the scalar variance or mean square fluctuation of  $\xi$ .  $c_\chi$  is an empirical constant taken to be equal to 2.0. Note that the convective term in  $\eta$  direction does not appear due to little differential diffusion in  $NO-O_3$  reaction system.

It is assumed that the reaction is irreversible as,



with the reaction rate  $w$  given as,

$$w = k_0 Y_{NO} Y_{O_3} \quad (21)$$

where  $k_0$  is the reaction rate constant,

$$k_0 = 0.37 \times (1 + 0.01 \times (T - 293.15)) \text{ (p.p.m.}^{-1} \text{s}^{-1}) \quad (22)$$

with  $T$  the fluid temperature in Kelvin.

The calculation domain is discretized in  $56 \times 31$  rectangular grids. In  $\eta$  space the grid spacing is dense near zero, unity and  $\xi_{stoic}$ , and sparse elsewhere. The number of grids is chosen as 41, 51 in  $\eta$  direction, respectively, according to the  $\xi_{stoic}$  values.  $\xi_{stoic}$  is the stoichiometric mixture fraction which is dependent on the inlet reactants and concentrations as,

$$\xi_{stoic} = \frac{0 - (Y_f - Y_{\alpha}/\xi_{st})_O}{(Y_f - Y_{\alpha}/\xi_{st})_F - (Y_f - Y_{\alpha}/\xi_{st})_O} \quad (23)$$

where  $Y_f$  and  $Y_{\alpha}$  are inlet fuel and oxidizer concentrations respectively,  $\xi_{st}$  is the stoichiometric coefficient for the overall reaction.

The flow field is taken as two-dimensional with free flow and adiabatic boundary. The conditional mean profiles are unknown at the nozzle exit plane ( $x=0$ ), with only the bounding mixture fraction ( $\eta=0,1$ ) being present, and are to be assumed for calculations. It is known that the form of the starting profiles appears to have no significant influence on calculated results. Then, the boundary treatment for the CMC equation is as following[7],

$$0 \leq \eta < \xi_{stoic} : Q_i(\eta) = (1 - \frac{\eta}{\xi_{stoic}}) Y_{i,O} + \frac{\eta}{\xi_{stoic}} Y_{i,pl} \quad (24)$$

$$\xi_{stoic} < \eta \leq 1 : Q_i(\eta) = \frac{1-\eta}{1-\xi_{stoic}} Y_{i,pl} + \frac{\eta-\xi_{stoic}}{1-\xi_{stoic}} Y_{i,F} \quad (25)$$

for chemical species  $i = 1, \dots, N$  at  $x = 0$ , i.e. at the nozzle exit plane, with  $Y_{i,pl}$  the pilot mass fraction defined as,

$$Y_{i,pl} = \frac{m_{i,total}}{m_{total}} \quad (26)$$

where  $m_{i, total}$  the mass flux of the species  $i$ , and  $m_{total}$  the total mass flux at the nozzle exit plane. The spatial boundary conditions for the CMC equation are given below,

$$\begin{aligned} Q_i(x) |_{\eta=0} &= Y_{i,O}(x) \\ Q_i(x) |_{\eta=1} &= Y_{i,F}(x) \end{aligned} \quad (27)$$

From above boundary treatment, the solution procedure for CMC formulation becomes a series of premixed reacting flow computations along  $\eta$  direction.

All the elliptic partial differential equations with the boundary conditions are integrated over the control volumes to obtain numerical solutions. The velocity, pressure and other dependent variables are stored in staggered positions on the finitely discretized grids. The SIMPLE algorithm is used to solve the equations. Because all the governing equations including the CMC equation are solved implicitly, the stiffness of the conditionally averaged species equations will not be a serious problem with the calculations numerically more stable.

There are several ways to calculate the pdf, such as the clipped Gaussian, Beta function, etc. with varying degrees of success. The conventional Beta function pdf is used here for its relative simplicity and flexibility in nonpremixed reacting flows. The Beta function pdf  $P(\xi)$  for the mixture fraction  $\xi$  has the form,

$$P(\xi) = \xi^{a-1}(1 - \xi)^{b-1}/\beta(a, b) \quad (28)$$

with

$$\begin{aligned} a &= f[f(1 - f)/g - 1] \\ b &= a(1 - f)/f \end{aligned} \quad (29)$$

$$\beta(a, b) = \int_0^1 \xi^{a-1}(1 - \xi)^{b-1} d\xi$$

where  $f$  is the mean value and  $g$  is the mean square fluctuation of  $\xi$ . With the use of Beta function pdf, conditional mean variables  $\varphi(\eta)$  are weighted to provide the unconditional mean variables  $\overline{\varphi}$  needed in the flow and mixing calculation,

$$\overline{\varphi} = \int_0^1 \varphi(\eta)P(\eta)d\eta \quad (30)$$

#### 4. RESULTS AND DISCUSSION

Figure 2 shows the calculated mean mixture fraction and its r.m.s. fluctuation  $f'$  profiles at  $x/M=16$  and 21 for the given experimental conditions.  $M$  is equal to 0.32m and  $\delta$  is the width of the mixing layer defined as the distance between the points where  $f=0.1$  and  $f=0.9$ . Note that there is not much scatter in calculation results for different Damkohler numbers, which is consistent with the experimental results and represents the passive reacting flow.

Figures 3 shows the results for the mass density averaged scalar  $\overline{Q}_i$ , normalized by the corresponding inlet species concentration. For finite Damkohler number  $N_D$ , the mean species concentration curves lie between the frozen and equilibrium limits and higher  $N_D$  will lead to mean concentration to be closer to the equilibrium values.

Figure 4 gives the relationship between  $Q_{O_2}$  and  $Q_{NO}$ , which shows that the

increase of  $N_D$  makes the curve tend to the left bottom corner. The measured joint pdf for the species concentrations[6] is close the curves in Fig. 4 with some scatter about the mean value. Figure 5 shows mean reaction rate  $\bar{w}$ . From above results, it is known that the present predictions are in good agreement with measurements.

Figure 6 and 7 show the normalized conditional averaged scalar  $Q_i$  and reaction rate  $w$  profiles with respect to  $\eta$ . The solid curve represents the case with Damkohler number  $N_D$  of 1.81, and the dashed curve with the  $N_D$  of 0.30. It can be inferred that a larger  $N_D$  results in a higher reaction rate and the maximum value occurs near the  $\xi_{stoc}$ .

In Fig. 8(a), the conditional averaged scalars are given at different transverse locations. It demonstrates some deviation between the curves, This effect becomes larger near  $\xi_{stoc}$ , which implies that the reduction of spatial dimensionality might involve some error even for this simple case. Note from Fig. 8 that, although the term  $\partial Q_i / \partial \eta$  varies remarkably respect to  $\eta$ , its derivatives to spatial coordinate  $x$ , or  $y$ , could be taken as negligible because there is not much scatter from the numerical results. This result numerically validates the assumption,  $\bar{\rho} D_i \langle \nabla \xi | \eta \rangle \cdot Q'_x \approx 0$ .

## 5. CONCLUDING REMARKS

(1) By taking into account the molecular and turbulent diffusion effects, the modified elliptic type CMC formulation is derived.

(2) A simplified solution procedure is proposed to reduce the computational burden due to the increased dimensionality of the conditionally averaged variables. Its implementation is under way.

(3) The modified CMC formulation is implemented to simulate a nonpremixed mixing layer. The calculated results show good agreement with measurements.

(4) The reduction of dimensionality and ignorance of diffusion terms will involve errors because the diffusion effect may be important in general problems.

(5) It is suggested that the CMC formulation considering molecular and turbulent diffusion effects be used in general elliptic problems.

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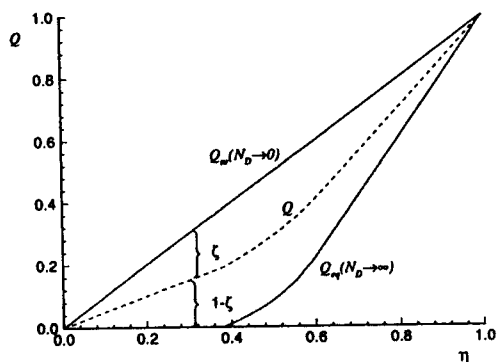


Fig.1 A simplified functional relationship of  $Q$  with respect to the reaction progress variable,  $\zeta$ . The dashed curve represents the linear weighted average of Eq.(17).

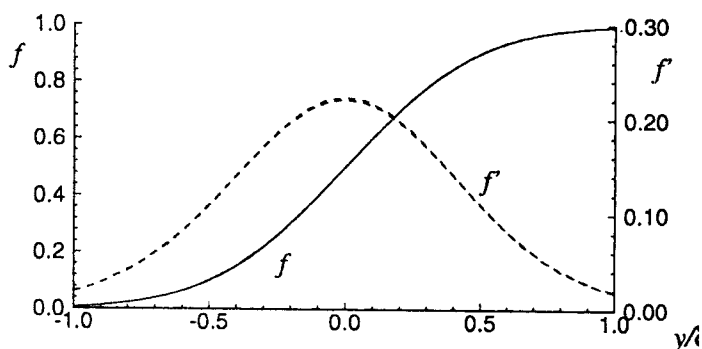
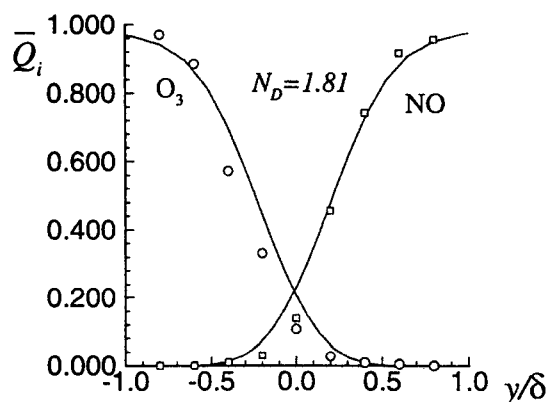
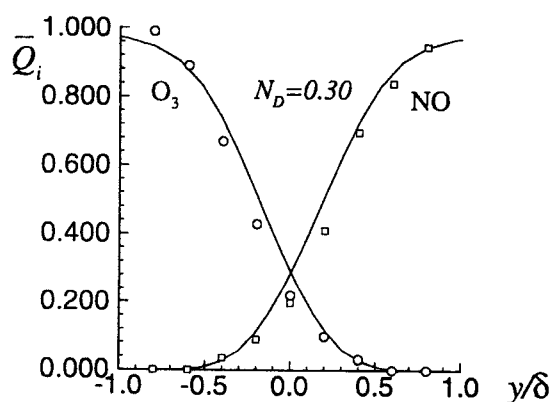


Fig.2 Profiles of mean mixture fraction  $f$  and its r.m.s. fluctuation  $f'$ .



(a)  $N_D = 1.81$



(b)  $N_D = 0.30$

Fig. 3. Normalized unconditional mean reactants concentration  $\bar{Q}_i$  at  $x/M = 21$ , symbols: measurements, lines: predictions.

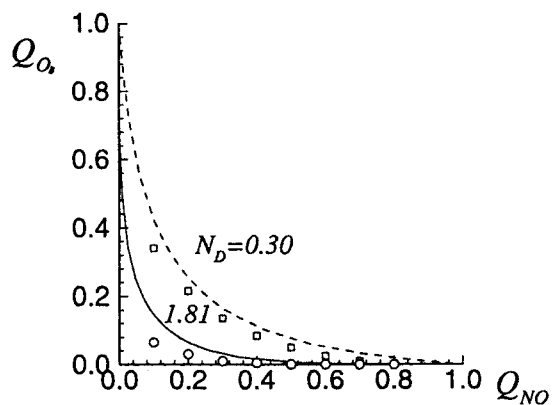


Fig. 4. Normalized conditional mean reactants  $Q_{O_3}$  vs.  $Q_{NO}$  relationship,  $x/M = 21$ ,  $y/\delta = 0.0$ .

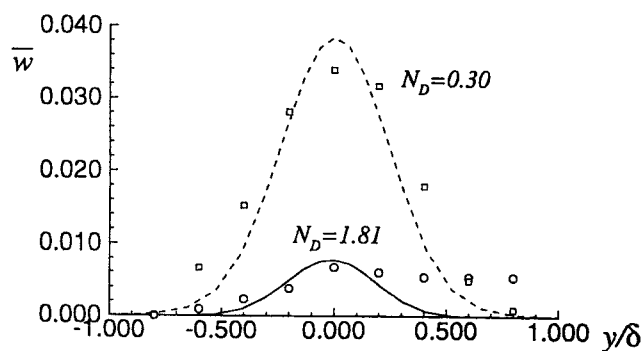


Fig. 5. Normalized mean reaction rate at  $x/M = 21$ , symbols: measurements.

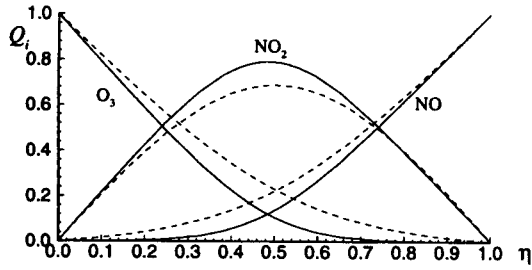


Fig. 6 Normalized conditional mean of species concentration,  $x/M = 21$ ,  $y/\delta = 0.0$ , for  $N_D$ : — 1.81, - - - 0.30.

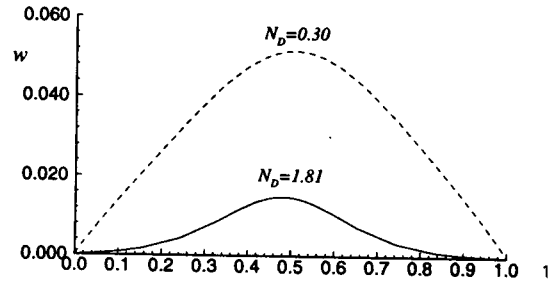
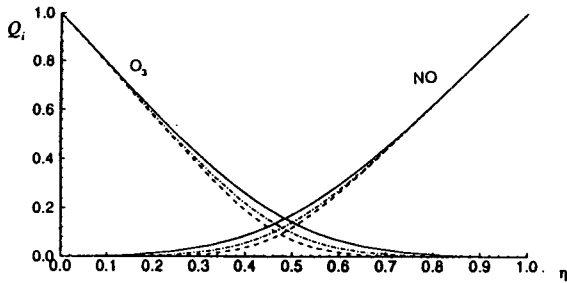
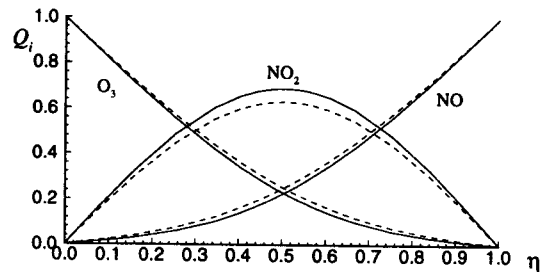


Fig. 7 Normalized conditional mean of the reaction rate,  $x/M = 21$ ,  $y/\delta = 0.0$ .



(a)  $x/M = 21$ , for  $y/\delta$ : — 0.0, - - - 0.2, ···· -0.2.



(b)  $y/\delta = 0.0$ , for  $x/M$ : — 21, - - - 12.

Fig. 8. Normalized conditional mean species concentrations  $Q_i$  at different monitoring locations,  $N_D = 1.81$ .