Third International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
10-12 December 2003

GLOBAL FLUCTUATION SECOND-ORDER MOMENT MODEL FOR TURBULENT REACTING FLOW IN GAS COMBUSTION

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ABSTRACT

The object of this study was to develop a mathematical model of turbulent reacting flows in gas combustion, comprising turbulent combustion reaction and NO_X formation. Different fluctuations and their influences on the Arrehenius reaction rate was estimated with second-order moment (SOM) method and a global fluctuation model was set up. The model closure was completed by a concept of turbulent density fluctuation intensity to be introduced and it's simulation model was set up. The analysis based on the earlier SOM models (Zhou, 2000) indicated that the proposed model will be more reasonable and economic for simulating the rate of combustion and NO_X formation.

NOMENCLATURE

A, B	pre-exponential factor
E	activation energy
g	mean square value of fluctuation
I	function defined in eq.(15)
k , K	reaction rate coefficient
M	molecular weight
p	pressure
R	universal gas constant
T	temperature
h	stagnation enthalpy
w	reaction rate
Y	mass fraction
Z	function defined in eq.(16)
ρ	density

Subscripts

re	reactant
pr	production
f	fuel
d	density
all	global fluctuation
j	fuel or NO_X

INTRODUCTION

There are two kinds of reactions in gaseous turbulent combustion flow: the faster or equilibrium combusting reaction and the slower or partial equilibrium NO_x formation reaction. Both of reactions are influenced by turbulent fluctuations, the influence mechanism is the effects of fluctuations of density, temperature and concentration on the Arrhenius model, and these effects are defined as the global fluctuation. However, the earlier studies focus on either applying all fluctuations to the conservation equations in differential form, for the velocity, temperature and concentration fields in turbulent combustion flows, and lead to a problem of more complex solution, or applying to the Arrehenius equation without considering the density fluctuation. Many experiments and researches suggest that the effect of density fluctuation increases obviously on NO_x formation in combusting turbulent flow(Muniz, 2001), and post-processing of these effects on Arrhenius rate equation is more and more adopted (Lau, 1995, Polifke, 1996). Second-order moment(SOM) turbulent-chemistry models that were reported can well simulate the turbulent combustion and NO_x formation (Zou, 2000), but the simulating results lead to under-predicting the value of NO_x formation as without considering the density fluctuation in combustion zone. This article describes the detailed fluctuations of density, temperature and concentration and has formed the global fluctuation SOM turbulent-chemistry models with post-processing method based on the earlier SOM models proposed by Zhou (2000).

MODEL DESCRIPTION

Analysis

The Arrehenius expression for the instantaneous production rate is

$$w_f = A\rho^2 Y_1 Y_2 \exp\left(-E/RT\right) \tag{1}$$

using Reynolds decomposition (Jones, 1982 and Smith, 1992) for the global fluctuating variables (ρ, T, Y_1, Y_2), eq. (1) becomes

$$\overline{w}_f = A\overline{\rho}^2 \overline{Y_1}\overline{Y_2} \exp(-E/\overline{RT})\left\{1+\frac{\overline{\rho'\rho'}}{\overline{\rho}\overline{\rho}}+\frac{\overline{Y_1'Y_2'}}{\overline{Y_1}\overline{Y_2}}+2\frac{\overline{\rho'Y_1'}}{\overline{\rho}\overline{Y_1}}+2\frac{\overline{\rho'Y_2'}}{\overline{\rho}\overline{Y_2}}\right.$$
$$\left.+\frac{E}{\overline{RT}}\left[\frac{\overline{Y_1'T'}}{\overline{Y_1}\overline{T}}+\frac{\overline{Y_2'T'}}{\overline{Y_2}\overline{T}}+\left(\frac{E}{2\overline{RT}}-1\right)\frac{\overline{T'^2}}{\overline{T}^2}\right]+\cdots\right\} \tag{2}$$

The introduced expression of SOM model has the limitation that requires $E/RT<1$. Otherwise, taking Taylor series expression for the exponential function in equation (2) may produce serious truncated errors, and the series converges very slowly. Thus the conventional

decomposition renders this approach intractable. Furthermore, the unknown correlations within the brackets such as $\overline{\rho^2}/\overline{\rho}^2$ lead to problems of closure even more complex. Pope (1977, 1981) has presumed a form for the joint probability density function (PDF). However, the presumed PDF suffers from the disadvantage that the number of moment equations increases very rapidly with the number of independent species present. Furthermore, the solution of PDF is difficult and needs big computer storage. All these methods were limited to application. For these, two simple approaches can be adopted. One method is SOM jointed simple PDF, but more than two simple PDF to be used such as $pdf(\rho)pdf(T)$ may bring error about 9% (Ishii, 2000). The other method is using the post-processing that based on the earlier SOM models of which without considering the density fluctuation, and the global fluctuation SOM model can be set up with density fluctuation considered by SOM decomposition of the density variable.

Background

Zhou (2000) set up different SOM models to simulating turbulent-chemistry interaction based on the Reynold expansion of Arrehenius instantaneous reaction rate eq.(1). Omitting density fluctuation ρ', the time-averaged reaction rate was obtained as

$$\overline{w}_f = \overline{A\rho^2 Y_1 Y_2 \exp(-E/RT)} = A\rho^2 \overline{kY_1Y_2}$$
$$= A\rho^2 \overline{(\overline{k}+k')(\overline{Y_1}+Y_1')(\overline{Y_2}+Y_2')} \quad (3)$$

or

$$\overline{w}_f = A\rho^2 \overline{(\overline{Y_1}+Y_1')(\overline{Y_2}+Y_2')\exp\left[-\frac{E}{R(\overline{T}+T')}\right]} \quad (4)$$

where, $k=\exp(-E/RT)$. Three versions of SOM closures have been set up on the bases of eq.(3) or eq.(4).

SOM Model-Version 1

Taking a series expansion for the exponential function in eq.(4), and assuming

$$\frac{E}{R\overline{T}}\frac{T'}{\overline{T}} << 1$$

the SOM model-version 1 is

$$\overline{w}_f = A\rho^2 \overline{Y}_1 \overline{Y}_2 \exp(-\frac{E}{R\overline{T}})[1+F] \quad (5)$$

where

$$F = \frac{\overline{Y_1'Y_2'}}{\overline{Y}_1\overline{Y}_2} + \frac{E}{R\overline{T}}\left(\frac{\overline{T'Y_1'}}{\overline{T}\overline{Y}_1} + \frac{\overline{T'Y_2'}}{\overline{T}\overline{Y}_2}\right) + \frac{1}{2}\left(\frac{E}{R\overline{T}}\right)\overline{\left(\frac{T'}{\overline{T}}\right)^2}$$

All of the second-order correlations of fluctuations are solved by the following transport equation

$$\frac{\partial}{\partial t}\left(\rho\overline{\varphi'\phi'}\right) + \frac{\partial}{\partial x_j}\left(\rho\overline{u}_j\overline{\varphi'\phi'}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_\varphi}\frac{\partial\overline{\varphi'\phi'}}{\partial x_j}\right)$$
$$+ c_1\mu_T\frac{\partial\overline{\varphi}}{\partial x_j}\frac{\partial\overline{\phi}}{\partial x_j} - c_2\rho\frac{\varepsilon}{k}\overline{\varphi'\phi'} \quad (6)$$

where φ, ϕ express Y_1, Y_2 and T, respectively.

SOM Model-Version 2

Based on eq.(3) and neglecting the third-order correlation, the time-averaged reaction rate of SOM model-version 2 is

$$\overline{w}_f = A\rho^2[(\overline{Y}_1\overline{Y}_2 + \overline{Y_1'Y_2'})k + \overline{Y}_1\overline{k'Y_2'} + \overline{Y}_2\overline{k'Y_1'}] \quad (7)$$

The exponential function k is obtained by simple PDF of $\overline{k} = \int \exp(-E/RT)p(T)dT$ for temperature to avoid the approximation by using series expansion.

SOM Model-Version 3

The exponential function k is obtained by simple PDF because of the error of series expansion when $E/RT > 1$, and it's fluctuation correlation was transformed into

$$\overline{k'Y'} = \overline{kY} - \overline{k}\overline{Y} = \iint kYp(Y)dTdY - \overline{Y}\int kp(T)dT$$

and the time-averaged reaction rate in version 3 is obtained as

$$\overline{w}_f = A\rho^2\overline{Y}_1\overline{Y}_2\exp(-E/R\overline{T})Z \quad (8)$$

where the function Z reflects the effects of turbulent fluctuations of T, Y_1 and Y_2 on the reaction rate

$$Z = ch\left(\frac{E}{R\overline{T}}\frac{g_T^{1/2}}{\overline{T}}\right)\left[1 + \frac{\overline{Y_1'Y_2'}}{\overline{Y}_1\overline{Y}_2} + \left(\frac{g_{Y1}^{1/2}}{\overline{Y}_1} + \frac{g_{Y2}^{1/2}}{\overline{Y}_2}\right)th\left(\frac{E}{R\overline{T}}\frac{g_T^{1/2}}{\overline{T}}\right)\right]$$

where

$$ch(x)=\left(e^x+e^{-x}\right)/2,\ sh(x)=\left(e^x-e^{-x}\right)/2,\ th(x)=sh(x)/ch(x)$$

The Thermal NO_x Formation Rate of Zeldovich Mechanism

The NO_x instantaneous formation rate in combustion flame was obtained as the same as previous SOM model-version 3 and new three presumed-PDFs finite rate models were set up (Zhou, 2000), the later models will produce more than 9% error by more than two simple PDF to be used (Ishii, 2000). Another researcher's NO_x instantaneous formation rate expression (Chen, 1992, Raine,1995) is adopted:

$$\overline{w}_{NO} = B\rho^{3/2}T^{-1/2}\exp(-E/RT)Y_{N_2}Y_{O_2}^{1/2} \quad (9)$$

where, B is a pre-exponent factor, E is the activation energy, which were given by Chen (1992) and Raine (1995).

DERIVATION OF GLOBAL FLUCTUATION MODEL

Derivation

Consider the equation of state in the form $p = \rho R_{NO}T$, $Y_{N_2} = Y_1$, and $Y_{O_2}^{1/2} = Y_{1/2O_2} = Y_2$, then

$$\overline{w}_{NO} = B(p/R_{NO})^{-1/2}\rho^2 Y_1 Y_2\exp(-E/RT) \quad (10)$$

For incompressible or micro-compressible gas flow, $p'=0$, and provided $p=\overline{p}=$constant, eq. (10) can be united to the universal form as that of combusting reaction model

$$\overline{w}_{NO} = A_{NO}\rho^2 Y_1 Y_2 \exp(-E/RT) \quad (11)$$

eq. (11) can be applied to all the above SOM model-versions and the others, and in which, by introducing the new representation of K as $\overline{K} = \overline{Y}_1 \overline{Y}_2 \exp(-E/R\overline{T})$

Hence

$$\overline{w}_{NO} = A\overline{\rho}^2 \overline{K} \quad (12)$$

The derivation of universal form (12) is adaptable to all SOM versions, not only to combustion reaction rate, but also to the NO_x formation rate. Expanding eq. (12) with SOM method by considering the density fluctuation, we find that post-processing the density fluctuation can modify the $\overline{w}_f$ or $\overline{w}_{NO}$ of all versions as $\overline{w}_{all}$, and the so called global fluctuation model can then be set up

$$\overline{w}_{all} = \overline{A\rho^2 \overline{K}} = A\overline{\rho^2}\,\overline{K} = A\overline{(\overline{\rho}+\rho')^2}\,\overline{K}$$
$$= A\overline{(\overline{\rho}^2 + 2\rho'\overline{\rho} + \rho'^2)}\,\overline{K} \quad (13)$$

Using Reynold's decomposition laws, the global fluctuation SOM model can be obtained as

$$\overline{w}_{all} = A\overline{\rho}^2 \overline{K}\left(1+\frac{\overline{\rho'^2}}{\overline{\rho}^2}\right) = \overline{w}_j\left(1+\frac{\overline{\rho'^2}}{\overline{\rho}^2}\right) \quad (14)$$

where, $j=f$, or NO. Unlike $\overline{T'T'}$ and $\overline{Y_1'Y_2'}$, that may be obtained by solving the eq. (6), how to simulate the $\overline{\rho'\rho'}$ term lead to a more difficult problem of closure.

Model Closure

This model closure becomes more tractable if a concept of turbulent fluctuation intensity be introduced to define the $\overline{\rho'^2}/\overline{\rho}^2$ as the concept of turbulent density fluctuation intensity I_d

$$I_d \equiv \sqrt{\frac{\overline{\rho'\rho'}}{\overline{\rho}\,\overline{\rho}}} \quad (15)$$

so

$$\overline{w}_{all} = \overline{w}_j(1+I_d^2) = \overline{w}_j Z_d \qquad (j=f,\ or\ NO) \quad (16)$$

where, $Z_d = 1+I_d^2$, the modified function factor Z_d, reflects the effect of density fluctuation on the reaction rate. Simulation of the I_d may close the global fluctuation model. Introducing the enthalpy equation

$$h = \int_0^T c_p\, dT + h_{pr}^0 Y_{pr}$$

and state equation of combustion mixture

$$p = \rho RT\left(\frac{1-Y_{pr}}{M_{re}} + \frac{Y_{pr}}{M_{pr}}\right)$$

Using Reynold's decomposition, the following equations obtained by Bray and Moss model (Bray and Moss, 1977)

$$T' = h_{pr}^0 Y_{pr}' / C_p \quad (17)$$

$$\rho' = -\overline{\rho}\Psi Y_{pr}' \quad (18)$$

where,

$$\Psi = \frac{h_{pr}^0}{c_p \overline{T}} + \frac{1/M_{pr} - 1/M_{re}}{(1-\overline{Y}_{pr})/M_{re} + \overline{Y}_{pr}/M_{pr}} \quad (19)$$

so, I_d can be deducted as

$$I_d^2 = \frac{\overline{\rho'^2}}{\overline{\rho}^2} = \Psi^2 \overline{Y_{pr}' Y_{pr}'} \quad (20)$$

where, $\overline{Y_{pr}' Y_{pr}'}$ can be solved by eq. (6) without additional transport equation and made the global fluctuation model closed. The obtained modeling eq. (19) reflects the effects of heat release, fuel type, concentration or mass fraction fluctuation, and shows analogy to the earlier research (Muniz, 2001).

CONCLUSION AND DISCUSSION

The global fluctuation models have united the combustion reaction model and thermal NO_x formation rate model as one form, the earlier form of reacting rate models w_f and w_{NO} may be modified by factor $Z_d=1+I^2_d$ when the density fluctuation to be considered. Hence, eq. (16), eq. (19) and eq. (20) composite the global fluctuation SOM model, comprising gas combustion reaction rate and thermal NO_x formation rate. particular, provided $\rho'=0$, then $I_d=0$, hence $w_{all}=w_j$, i.e. the original SOM models ($j=f,NO$) recovers from the global fluctuation model. The results of globe fluctuation model lead to the following conclusions.

(1) The global fluctuation model developed here, is an extension of second-order moment turbulence-chemistry models. This results in a particularly efficient formulation, when density fluctuating within combustion zone. The earlier investigations showed the lower predictions of NO_x (Zhou, 2000). However, the global fluctuation models may lead to increase the NO_x predicting values more close to that of measured. Because of the modifying factor Z_d satisfies $Z_d=1+I_d^2>1$, and the experimental result of the maximum density fluctuation I_d^2 is 33% (Bill, 1982). Hence, $\overline{w}_{all} > \overline{w}_{NO}$, which makes the value of source term $\overline{w}_{all}$ in NO_x transport equation increased and predicts the correct tendency of NO_x formation.

(2) The concept of density fluctuation intensity and it's modeling made the globe fluctuation model closed and need not increasing computation time and storage because of no extra transport equation to be solved. This may be adapted to the post-processing method to simulate the NO_x formation.

REFERENCE

MUNIZ L., MUNGAL M.G., (2001), "Effect of heat release and buoyancy on flow structure and entrainment in turbulent non-premixed flames", *Combustion and Flame*,126, 1402-1420.

LAU J. H. W., (1995), "Comparison of pdf and eddy-dissipation combustion models applied to a propane jet flame", *Combustion and Flame*, 102, 209-215.

POLIFKE W., DÖBBELING K., (1996), "Sattelmayer T. et al. A NO_x prediction scheme for lean-premixed gas

turbine combustion based on detailed chemical kinetics", *Journal of Engineering for Gas Turbine and Power*, 118, 765-772.

ZHOU L. X., CHEN X. L., ZHENG C. G. ET AL., (2000), "Second-order moment turbulent-chemistry models for simulating NO_x formation in gas combustion", *Fuel*, 79, 1289-1301.

JONES W. P., WHITELAW J. H., (1982), "Calculation methods for reacting turbulent flows: a review", *Combustion and Flame*, 48, 1-26.

SMITH D. A., COX G., (1992), "Major chemical species in buoyant turbulent diffusion flames", *Combustion and Flame*, 91, 226-238.

POPE S. B.,(1977), "The implications of the probability equations for turbulent combusting flows", *Combustion and Flame*, 29, 235.

POPE S. B., (1981), "A Monte Carlo method for the p.d.f. equation of turbulent reactive flow", *Combustion Science and Technology*, 25, 159-174.

ISHII T., ZHANG C., SUGIYAMA S., (2000), "Effect of NO models on the prediction of NO formation in a regenerative furnace", *Journal of Energy Resources Technology*, 122, 224-228.

CHEN J. Y., KOLLMAN W., (1992), "PDF modeling and analysis of thermal NO formation in turbulent non-premixed hydrogen-air jet flames", *Combustion and Flame*, 88, 397-412.

RAINE R. R., STONE C. R., (1995), "Gould J. Modeling of nitric oxide formation in spark ignition engines using a multi-zone burned gas", *Combustion and Flame*, 102, 241-250.

BRAY K. N. C., AND MOSS J. B., (1977), "A unified statistical model of the premixed turbulent flame", *Acta Astronaut*, 4, 291-319.

BILL R. G., JR, NAMER I., AND TALBOR L.,(1982), "Density fluctuation of flame in grid-induced turbulence", *Combustion and Flame*, 44, 277-285.