Final Programme

02-05 April 2002 – Estoril – Portugal
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<td>KEYNOTE ADDRESS: INFU SETTING THE SCENE, Prof. John Ward</td>
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<td>KEYNOTE LECTURE: INTELLIGENT COMBUSTION CONTROL, FROM MYTHS TO REALITY — Dr. Jean Bernard Michel</td>
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A SMALL EXHIBITION OF TECHNICAL AND COMMERCIAL LITERATURE WILL BE RUN IN PARALLEL WITH THE POSTER SESSIONS
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SIMULATION OF BUBBLING FLUIDISLED BED GASIFIERS
S. HAMEL, F. MINTUS, H. HASSELBACK AND W. KRUMM
UNIVERSITAT SIEGEN (GERMANY)

NUMERICAL SIMULATIONS OF CEMENT KILN FIAMES
R. WEBER, D. BRAUCKMANN, R. SCHOLZ, M. MÄNNCHI AND W. KAMP
INSTITUT FÜR ENERGIEVERBRAUCHSTECHNIK UND BRENnstofftechnIK DER TU Clausthal (GERMANY) AND INTERNATIONAL FLAME RESEARCH FOUNDATION (HOLLAND)

PREDICTION OF BILLET TEMPERATURE BY THE TOTAL HEAT EXCHANGE FACTOR IN REHEATING FURNACE
RESEARCH INSTITUTE OF INDUSTRIAL SCIENCE & TECHNOLOGY (KOREA)

MODELLING OF THE STATE OF TWO-PHASE FLOW "DROPLETS-GAS"
G. MILAUSKAS, V. LUKOSYČIUS AND V. SAVELSKIS
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O. SILVA AND P.J. COELHO
UNIVERSITY OF ÉVORA AND INSTITUTO SUPERIOR TECNICO (PORTUGAL)

A TRANSIENT, MULTI-DIMENSIONAL, ZONE MODEL OF A ROLLER KILN USED FOR FIRING CERAMIC TILES
J.A. SOUTA, S.C. CORREIA, J. WARD AND M. NOGUEIRA
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NUMERICAL MODELLING OF THE HEATING CHAMBER OF A CONTINUOUS ANNEALING LINE
F.J. FERNANDEZ, M.M. PRIETO, J. DÍAZ, I. SUAREZ AND J.L. PRIQUELES
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NUMERICAL MODELLING OF HIGH TEMPERATURE AIR "FLAMELESS" COMBUSTION
V.I. Golovitchev AND R. Jarvishi
CHALMERS UNIVERSITY OF TECHNOLOGY (SWEDEN)

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M. MARKLAND AND R. EBART
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UNIVERSITY OF GLAMORGAN (UK)

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UNITED KINGDOM
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S. PATUMSAWAD AND K. KUFF.E
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R. BECHARRY AND T.R. BOTT
THE UNIVERSITY OF BIRMINGHAM (UK) AND UNIVERSITY OF MAURITIUS (MAURITIUS)

ALTERNATIVE FUELS FOR SUPPLEMENTARY FIRING ADD VALUE AND FLEXIBILITY TO COMBINED CYCLE AND COGENERATION PLANTS
A.E. BATTISON AND J. C. BACKLUND
COEN COMPANY, INC. (USA)
INTEGRAL MODEL FOR SOOT FORMATION CALCULATION OF TURBULENT DIFFUSION FLAMES IN INDUSTRIAL FURNACES

BUI VAN GA - University of Danang
LE VAN LU - Ho Chi Minh City University of Technology

ABSTRACT

Turbulent diffusion flames are widely used in industry because of their safety. Nevertheless, their efficiency and the pollution emission depend on the organization of the combustion medium and this fact needs knowledge of the structure of the flame. The experimental measurement of the instantaneous and local values of oxygen and fuel is very difficult, and sometimes is impossible inside the combustion chamber. So the prediction by the mathematical model is very helpful.

In this paper a model for calculating the soot formation in turbulent diffusion flames is presented. The turbulent nonpremixed combustion process is modeled via the conserved scalar model where the fraction mixture f is chosen as conserved scalar. The soot formation is calculated via the Tesner-Magnussen model. The equations system is closed by k- turbulence model. The results given by the model is validated against experimental data on propane and gasoline flames.

KEYWORDS

Model calculation, soot formation, turbulent diffusion flames, combustion, industrial furnaces.

1. INTRODUCTION

The modeling of flow in reaction medium is very complex because of the variations of species concentrations and of the energy release. The rigorous calculation should be carried out with a multidimensional configuration and it requests the kinetics of each element chemical reaction. This is a very hard task and we need a very high performance computer. The development of numerical simulation of combustion based on fast reaction hypothesis allows us to simplify this problem in prediction of combustion phenomena, particularly in diffusion flames.

Before 1970, the numerical model based on the principle didn't examine the concentration fluctuations. However it was widely used in a lot of practical combustion systems. Howe and Shipman [1] suggested in 1965 a model named "rate of combustion" in which the reaction zone is simulated by bulbs of unburned gas dispersing in burned gas or conversely. The essential problem of this model is to establish the law of distribution of bulbs in flow.

During the 1970s years, Spalding presented his "eddy-break-up" model [2]. The basis of this model is the conception of reactivity. The rate of combustion depends on the reactivity and that
of transformation of big structures to small structures, i.e. rate of dissipation of eddies such as the heat transfer and rates of chemical reactions are considerable.

The "eddy dissipation" model of Magnussen [3], is established by a similar principle to the "eddy-break-up" model. In this model the rate of combustion is calculated via mean concentrations but not via the instantaneous values. In a turbulent diffusion flame, the chemical reaction is very fast so the combustion rate can be calculated via the rate of mixing between the oxygen and the fuel in molecular scalar, i.e. the rate of dissipation of eddies $\varepsilon / k$.

The above models allow us to calculate the rate of consumption of fuel so that we can determine heat release rate and other combustion parameters. But the model gives us the mean values. The fine analysis of diffusion combustion phenomena needs instantaneous and local values. Thus a new model has been developed and widely used in diffusion combustion: the conserved scalar model. In this model, one suggests that all species have the same effective diffusion and one conserves the hypothesis of an infinitely fast chemical kinetic because in a lot of cases the reaction rate is much higher than that of mixing between fuel and air. The thermodynamic state of mixture which is characterized by the species concentrations, fluid density and temperature, can be determined via a conserved scalar. The conserved scalar is a frozen term i.e. there is no source term in its conservation equation. The mixture fraction is often used as the conserved scalar. In this paper we will develop this model to calculate the soot formation in turbulence diffusion flames.

2. MODELING OF DIFFUSION COMBUSTION BY CONSERVED SCALAR MODEL

In case of diffusion flames, fuel and oxygen come from two different sources. The mixture fraction is defined as:

$$f = \frac{M_1}{M_1 + M_o} \quad (1)$$

where $M_1$ and $M_o$ are masses of fluid which come from fuel (1) and air (o).

According to this definition, the mixture fraction is conserved, i.e. it is frozen in combustion medium. In turbulent flame, because fuel and air concentrations are random quantities, so $f$ is also a random quantity in time and in space. The simplest way to calculate its value is to introduce a probability density function $P(f)$ of $f$. The pdf can be identified by mean value of $f$ and its variance $f^{n2}$ and they are the solutions of the following equations system [4]:

$$-\rho U \frac{\partial f}{\partial x} + \rho V \frac{\partial f}{\partial t} = 1 \frac{\partial}{\partial t} \left( \mu_1 \frac{\partial f}{\partial \tau} \right) \quad (2)$$

$$-\rho U \frac{\partial f^{n2}}{\partial x} + \rho V \frac{\partial f^{n2}}{\partial \tau} = 1 \frac{\partial}{\partial \tau} \left( \mu_1 \frac{\partial f^{n2}}{\partial \tau} \right) + c_{r1} \mu_1 \left( \frac{\partial f}{\partial \tau} \right)^2 - \frac{c_{r2}}{c_p} \rho e f^{n2} \quad (3)$$
One of the most important problems in conserved scalar model is the choice of pdf. There are many functions which have been used in the literature such as the Beta function, Gauss function, or Polynomial function. The figure 1 shows the polynomial pdf with n=1 in different cases.

![Figure 1: Forms of polynomial pdf in different cases](attachment:figure1.png)

As we have explained previously, the instantaneous values of species concentrations, the temperature and the fluid density can be calculated via the mixture fraction f. In general, the mean value and the fluctuations of a dependant variable (f) are determined respectively by the two following expressions:

$$\overline{f}^n = \int \left[ \overline{\phi(f)} \right]^n \cdot P(f) df$$

The experimental data of [8] show that the functions (f) for concentrations, temperature and density are not linear. For simplifying the calculation, we use linear approach for the relations (fig. 2) like that have been used in [7], [9]:

For temperature, because of the presence of a radiation term in the energy conservation equation the establishment of a relation between real temperature and conserved scalar is impossible. Crawford [12] proposed a formula for calculation of the real temperature of the gas via the adiabatic temperature:

$$T(f) = T_{ad}(f) \left( 1 - \chi \frac{T_{ad}(f)}{T_{ad,max}} \right)$$

![Figure 2: Linear relations Y_{ad}(f), Y(f) and T_{ad}(f)](attachment:figure2.png)
3. MODELING OF SOOT PRODUCTION

Soot formation

Soot is produced by intermediary of the HAP. The schema of HAP formation kinetic contains about 1000 elementary reversible reactions. The complete resolution of the equations system requires a heavy calculation which is not suitable for practical applications. A simple kinetic model is thus preferable.

According to Tesner [3], soot is formed via two stages: first, nucleus formation and second, soot formation basing on the nucleus concentration. The nucleus formation rate is written as:

\[ R_{nf} = n_o + (f_b - g) n - g_o n N \]  \hspace{1cm} (7)

In this formula:

- \( n_o \): Rate of nucleus formation depending on fuel concentration:
  \[ n_o = a_o c_f \exp\left(\frac{-E}{RT}\right) \]  \hspace{1cm} (8)
- \( a_o \): Constant.
- \( c_f \): Fuel fraction (kg/m\(^3\)).
- \( E \): Activation energy.
- \( R \): Universal gas constant.
- \( T \): Gas temperature.
- \( f_b \): Coefficient of line branch.
- \( g \): Coefficient of line termination.
- \( g_o \): Coefficient of termination of soot particles.
- \( n \): Nucleus concentration (part/m\(^3\)).
- \( N \): Soot particles concentration (part/m\(^3\)).

The rate of soot particle formation is:

\[ R_{s,f} = m_p (a - b N) n \]  \hspace{1cm} (9)

where

- \( m_p \): Mass of soot particle (kg/part).
- \( a, b \): Constants.

Soot combustion

Basing on the same principle of fuel combustion, Magnussen [3], proposed an eddy-dissipation model applied for soot combustion in which the rate of soot oxidation is written as:
Where

\[ A \] : Constant

\[ c_s \] : Soot concentration (kg/m\(^3\)).

\[ k \] : Turbulence kinetic energy (m\(^2\)/s\(^2\)).

\[ \varepsilon \] : Rate of Turbulence kinetic energy dissipation (m\(^2\)/s\(^3\)).

This relation is applied in the zone where soot concentration is lower than that of oxygen. If the soot concentration is higher, the soot combustion rate is:

\[
R_{s,c} = A \cdot c_s \left( \frac{\varepsilon}{k} \right) (\text{kg.m}^{-3}\text{s}^{-1}) \quad (10)
\]

\[
R_{s,c} = A \cdot \frac{c_{O_2}}{r_s} \left( \frac{\varepsilon}{k} \right) \left( \frac{c_s r_s}{c_s r_s + c_f r_f} \right) (\text{kg.m}^{-3}\text{s}^{-1}) \quad (11)
\]

\[ r_s, r_f \] are respectively the required oxygen mass for combustion of 1 kg of soot and fuel (kg/kg); \( c_{O_2} \) is oxygen concentration (kg/m\(^3\)).

Soot combustion rate is the lowest value between \( R_{s,c} \) given by (10) and (11). Soot production rate is finally determined by:

\[
R_s = R_{s,f} - R_{s,c} \quad (\text{kg.m}^{-3}\text{s}^{-1}) \quad (12)
\]

4. SET OF EQUATIONS

The main part of the set of differential equations for turbulent diffusion flames can be found in a paper of Tamanini [6] or Cook [9]. In the present work, we modify this set of equation by adding the soot formation model of Tesner-Magnussen.
\[
\begin{align*}
\frac{d\bar{m}}{d\bar{x}} &= \mu \left( \mu + \mu_r \right) \\
\frac{dW}{d\bar{x}} &= g_c (\rho - \langle \rho \rangle) \pi R^2 \\
\frac{d(kn)}{d\bar{x}} &= P_k + G_k - D_k \\
\frac{d(\bar{m}f_{\text{m}}^2)}{d\bar{x}} &= \epsilon \left( c_{e1} P_k + c_{e3} G_k - c_{e2} D_k \right) \\
\frac{d(\bar{m}N)}{d\bar{x}} &= R_N \\
\frac{d(\bar{m}S)}{d\bar{x}} &= R_s
\end{align*}
\]

In the above set of equations:

- $\bar{m} = 2\pi \langle \rho \rangle \int_0^\infty U(r) r dr$ and $W = 2\pi \langle \rho \rangle \int_0^\infty (U(r))^2 r dr$ (14)

- $\mu_r$ is the classical turbulent viscosity, given by: $\mu_r = c_{\mu} \langle \rho \rangle \frac{k^2}{\epsilon}$

- $\langle \rho \rangle$ is the radial average density considered as independent of radial distance $r$, ("Top-hat profile" hypothesis [9])

- $R$ is the radius of the jet given by [6]:
  \[
  R = \frac{\bar{m}}{\sqrt{\pi \langle \rho \rangle W}}
  \]

- $P_k$ is the kinetic energy production term given from mean velocity profile by integration:
  \[
  P_k = 2\pi \mu \int_0^\infty \left( \frac{dU(r)}{dr} \right)^2 r dr
  \]

- $G_k$ is a kinetic energy production term due to buoyancy [6]:
  \[
  G_k = g_c c_{\mu} \pi R^2 \sqrt{k \rho''^2}
  \]

- $D_k$ is the kinetic energy dissipation term:
  \[
  D_k = \langle \rho \rangle \epsilon \pi R^2
  \]
These equations can be deduced from the classical k-ε model in radial coordinates, with boundary layer hypothesis. Top-Hat profiles are assumed from all quantities except the velocity which is given by a two parameter Gaussian profile:

\[ U(\eta) = U_c \cdot \exp\left(-\ln(2) \cdot \eta^2\right) \]

with \( U_c \): axial velocity
and \( \eta \): undimensional radius relative to half velocity radius: \( \eta = \frac{r}{r_{0.5}} \)

Integration of the Gaussian velocity profile gives:

\[ U_c = \frac{2 \cdot W}{\pi} \quad \text{and} \quad r_{0.5} = \sqrt{\frac{\ln(2)}{2 \cdot \pi \cdot \rho \cdot W}} \quad (19) \]

The effective radius is then:

\[ R = \sqrt{\frac{2}{\ln(2)}} \cdot r_{0.5} \quad (20) \]

The kinetic energy production term is easily integrated to:

\[ P_k = \pi \cdot \frac{U_c^3}{\epsilon} \]

The initial conditions for \( k, \epsilon, f'' \) are determined from the nozzle exit values by:

\[ k = \alpha_k \cdot U_i^3 \quad ; \quad \epsilon = \alpha_\epsilon \cdot \epsilon_{\text{equilibrium}} \quad ; \quad f'' = 0 \quad (21) \]

\( \epsilon_{\text{equilibrium}} \) is calculated from \( k \), so that there is equality of production and dissipation terms in the kinetic energy balance. The main combustion rate is generally performed with the rectangular pdf. The computation is carried out on a Pentium III PC and the code is written in Pascal language. A fourth order Runge-Kutta method is used to solve the system of differential equations.

5. EXPERIMENTAL CONDITIONS

The model is tested by experimental data in turbulence diffusion flames of propane and gasoline. The experimental conditions are as follows:

<table>
<thead>
<tr>
<th>Flames</th>
<th>Nozzle diameter (mm)</th>
<th>Initial flow (l/h)</th>
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<tbody>
<tr>
<td>Propane</td>
<td>3</td>
<td>560</td>
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<tr>
<td>Gasoline</td>
<td>0.1</td>
<td>2.89</td>
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The soot fraction in the flame is measured by the light scattering method [10]. Gas concentrations are obtained by INTERMAT IGC-130 analysis instruments [13], [17].

6. RESULTS AND DISCUSSIONS

The choice of constants for the set of equations was discussed in our previous paper [14]. The results were used in this work. The figure 3 presents a comparison of fuel concentrations given by Beta, 1st order and 2nd order polynomial pdf. This figure shows that the difference of fuel concentrations given by the three pdf is low for high values (higher than about $10^{-3}$) of concentrations. In the higher part of flame, the fuel concentration given by the polynomial pdf falls quickly, however, that given by beta pdf decreases regularly.

Because of limitation of the precision of the instruments, the concentrations of fuel in higher part of the flame is not justified. We will pursue our research with more performance instruments for a more rigorous analysis. With a sufficient precision, we can use the polynomial pdf for simplifying the calculation. The following results are given by 1st order polynomial pdf.

The figures 4 and 5 show that the results given by the model with 1st order polynomial pdf fit well to the experimental data of oxygen and fuel concentrations.

Figure 6 gives a comparison of soot fractions in propane turbulence diffusion flame calculated by beta pdf and 1st order polynomial pdf. In this calculation the soot formation of Magnussen was used. Because soot formation is proportional to the fuel concentration so the beta pdf gives a soot fraction lightly higher than that given by the polynomial pdf. The comparison between model and measure of soot fraction in gasoline flame is represented on the figure 7.
7. CONCLUSIONS

The conserved scalar model that is first established for calculation of turbulent diffusion flames in the air was successfully developed to calculate the soot formation by an integral model.
The effect of pdf form used in the model on the results is not important. So we can use practically the 1st order polynomial pdf to simplify the calculation. A software based on the results can be made for pollution emission calculation of combustion in industrial furnaces.

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