

## Application of the One-Dimensional Model UPMFIRE to Calculate Jet Fire Characteristics and its Interaction with Obstacles

A. Crespo<sup>a</sup>, J. Servert<sup>a</sup>, J. Hernández<sup>b</sup>

<sup>a</sup> Departamento de Ingeniería Energética y Fluidomecánica, E.T.S.Ingenieros Industriales, UPM, José Gutiérrez Abascal, 2 - 28006 Madrid, Spain

<sup>b</sup> Departamento de Mecánica, E.T.S.Ingenieros Industriales, UNED, Ciudad Universitaria, 28040 Madrid, Spain

A one-dimensional model is applied to evaluate the interaction of turbulent jet diffusion flames of natural gas with engulfed obstacles. The fluid dynamics equations are complemented with models for chemical reaction, thermal radiation and an adaptation of the  $k$ - $\epsilon$ - $g$  closure method. The numerical results obtained for the radiation heat flux to engulfed vertical and horizontal cylinders and to nearby horizontal surfaces, and for the temperature distribution in the flame are compared with full-scale and wind-tunnel experimental results, and with those of a three-dimensional numerical model. In general, the results seem to be in good agreement, and UPMFIRE can be considered as a useful tool in risk assessment and in the design of flares.

### 1. INTRODUCTION

Turbulent jet fires are involved, either as a hazard or as a result of a controlled relief of flammable gases, in some operational or emergency situations. To design and operate some industrial installations where jet fires can occur, information about the heat transferred to surroundings objects or engulfed obstacles is needed. There are different ways to predict the effects of these fires. One is to use mathematical models based on the Navier-Stokes equations, complemented with some appropriate models describing the combustion and a closure procedure to model the turbulent transport terms. The numerical resolution of these models is commonly based on finite-differences approximations of the equations (Fairweather et al., 1992; Hernández and Crespo, 1994), which may require a relatively large computational effort.

If a jet center line and self-similar profiles in planes normal to it can be defined, the partial differential equations may be converted to ordinary differential equations, with the distance along the center line as the independent variable. The computer time to solve the problem is then substantially reduced, from hours to fractions of minutes. This type of one-dimensional (integral) model has been used extensively by Escudier (1972), Fay (1973), Tamanini (1981), Peters and Göttgens (1991), Cook (1991), and Caulfield et al. (1993), among others. In this work, the model UPMFIRE, developed by the authors, is compared with some experimental results. A more detailed description of the derivation of this model can be found in Servert

(1993). Fay (1973) proposed a model somehow similar to ours, although it has a more complex interpretation and introduces a definition of the average quantities that depends on the existence of an ambient wind, while UPMFIRE applies to any ambient flow conditions.

Whereas other models (Escudier, 1972; Tamanini, 1981; Cook, 1991; Caulfield et al., 1993) either assume top-hat profiles or sine-type profiles that end at a finite distance from the center line, UPMFIRE can also use self-similar profiles that extend to infinity in the transverse direction.

The three-dimensional equations describing the flow field are formulated assuming that the flow is parabolic along the center line. The k-ε-g model is used to close the turbulent equations, and relations for the mixture fraction and its variance are introduced.

The combustion model is based on an infinitely-fast reaction assumption and a prescribed shape for the probability-density function of the mixture fraction. The mass fractions of fuel, carbon dioxide and water vapor are obtained as functions of the mixture fraction and its variance, and the temperature is determined as a function of these same variables and of the enthalpy. A method similar to the one proposed by Caulfield et al. (1993) is used to calculate the mass fraction of soot.

The one-dimensional model can take into account the existence of engulfed obstacles, small in comparison with the characteristic length of the flame, through a finite jump in the flow conditions.

Finally, a comparison is made with wind-tunnel experimental results (Verheij and Duijm, 1991; Duijm, 1993) and with full-scale measurements (Ott, 1991; Bennett et al., 91). The model has also been compared with a three-dimensional model (Hernández and Crespo, 1994).

## 2. GOVERNING EQUATIONS

### 2.1. Three-dimensional equations

The one-dimensional model will be derived from the Favre-averaged, three-dimensional conservation equations of mass, momentum, energy, mixture fraction, turbulent kinetic energy, dissipation rate of the turbulent kinetic energy, and variance of the mixture fraction (Hernández and Crespo, 1994), which may be written in the general form

$$\nabla \cdot (\bar{\rho} \vec{v} \tilde{\phi} - \vec{\Gamma}_\phi) = S_\phi, \quad (1)$$

where  $\phi$  can be equal to: 1, any component of the velocity,  $\vec{v}$ , total enthalpy,  $h$ , mixture fraction,  $\xi$ , turbulent kinetic energy,  $k$ , dissipation rate of the turbulent kinetic energy,  $\epsilon$ , or variance of the mixture fraction,  $g$ . In this equation,  $\rho$  is the density and  $S_\phi$  is the source term. The Favre average is denoted by a tilde and the temporal average by a dash. The diffusion vector (except for the velocity components, for which some additional terms appear) is expressed as

$$\vec{\Gamma}_\phi = \frac{\mu_t}{\sigma_\phi} \nabla \tilde{\phi}, \quad (2)$$

where  $\mu_t$  is the turbulent dynamic viscosity, and  $\sigma_\phi$  is the turbulent Prandtl number for the variable  $\phi$ . The turbulent viscosity is obtained from

$$\mu_t = C_\mu \bar{\rho} \frac{k^2}{\varepsilon}, \quad (3)$$

where  $C_\mu = 0.09$ .

The source terms include buoyancy effects in the vertical momentum equation, thermal radiation in the energy equation (in which gravity has been neglected and the Mach number is assumed to be low), and production and dissipation terms in equations for  $k$ ,  $\varepsilon$  and  $g$ .

The model is completed with a perfect gas law and the state equation for enthalpy.

### 2.1. Combustion model

To define the combustion model, the classical hypothesis of one-step, irreversible reaction, represented by [Fuel +  $r_c$  Oxidizer  $\rightarrow$  (1+ $r_c$ ) Products] (where  $r_c$  is the stoichiometric ratio), fast chemistry, and equal diffusivities for all the species are made. This leads to the classical conserved-scalar approach and to the well known relation.

$$Y_F(\xi) = \frac{\xi - \xi_s}{1 - \xi_s}, \quad \xi > \xi_s \quad (4)$$

$$Y_F(\xi) = 0; \quad \xi \leq \xi_s,$$

where  $Y_F$  is the fuel mass fraction and  $\xi_s$  is the stoichiometric mixture fraction. From the instantaneous value, the Favre average is obtained through

$$\tilde{Y}_F = \frac{1}{1 - \xi_s} \int_{\xi_s}^1 (\xi - \xi_s) P(\xi) d\xi, \quad (5)$$

where  $P(\xi)$  is the Favre-averaged probability density function of  $\xi$  of a predefined shape, whose parameters are expressed in terms of the average value of the mixture fraction and  $g$ . An alternative approach is the use of a correlation for the unmixedness integral (Mudford and Bilger, 1984).

The mass fractions of oxidizer and products are

$$\tilde{Y}_p = (r_c + 1) (\xi - \tilde{Y}_F), \quad (6)$$

$$\tilde{Y}_O = (r_c \tilde{Y}_F + \tilde{Y}_{Oa}) - \xi (r_c + \tilde{Y}_{Oa}), \quad (7)$$

where the subscript a represents ambient conditions.

The products are mainly  $H_2O$  and  $CO_2$ , whose mass fractions are obtained from the stoichiometry. Other products are assumed to have small mass fractions, and are not relevant except for soot, which is taken into account because it plays an important role in radiative processes. The calculation procedure of the soot mass fraction can be seen in Caulfield et al. (1993).

If the specific heat at constant pressure,  $c_p$ , and the heat of reaction,  $Q$ , are assumed to be constant, enthalpy and temperature are related through

$$\tilde{h} = c_p \tilde{T} + Q \tilde{Y}_F \quad (8)$$

This relationship is used to obtain temperature from enthalpy and fuel mass fraction.

### 2.3. Ambient flow

The ambient flow where the jet diffuses corresponds to the surface layer of the atmospheric boundary layer in uniform, flat terrain. In this model, the ambient magnitudes satisfy equation (1) and are considered to change only with height (Servert, 1993).

## 3. DERIVATION OF THE ONE-DIMENSIONAL EQUATIONS

### 3.1. Definition of the spatial averages

One-dimensional models are based in the existence of self-similar axisymmetric profiles for the dependent variables of equation (1), such as

$$\tilde{\phi} - \phi_a = (\phi_0 - \phi_a) \psi_\phi \left( \frac{r}{R} \right) \quad (9)$$

where  $\psi_\phi$  satisfies

$$\int_0^\infty \psi_\phi 2\pi r dr = \pi R^2, \quad \psi_\phi(0) = 1. \quad (10)$$

$R$  and  $\phi_0$  are the parameters of the spatial distribution, which are functions of the coordinate along the flame, and  $r$  is the radial coordinate. The Gaussian distribution  $\psi(r/R) = \exp[-(r/R)^2]$  is the one used to obtain the results presented in this work.

These profiles are used to evaluate the following spatial-averages:

$$\dot{m} \langle \tilde{\phi} \rangle - \phi_a \dot{m} = \lim_{A \rightarrow \infty} \int_A \bar{\rho} \bar{u} (\tilde{\phi} - \phi_a) dA, \quad (11)$$

where  $\bar{u}$  is the velocity component normal to a surface,  $A$ , normal to the center line of the flame, in which the average of the velocity component contained in it,  $\langle \bar{w} \rangle$ , is equal to zero.

The mass flow rate,  $\dot{m}$ , across  $A$  is defined by

$$\dot{m} - \dot{m}_a = \lim_{A \rightarrow \infty} \int_A (\rho \bar{u} - \rho_a v_a \cos \theta) dA, \quad (12)$$

where

$$\dot{m}_a = \dot{m} \frac{\rho_a v_a \cos \theta}{\langle \rho \rangle \langle \bar{u} \rangle}, \quad (13)$$

and  $\theta$  is the angle that the normal to the surface  $A$  forms with the horizontal plane.  
The average density is defined using an equation of state

$$\langle \bar{\rho} \rangle = \frac{P_a}{R_g \langle \tilde{T} \rangle}, \quad (14)$$

where  $p_a$  is the ambient pressure,  $R_g$  is the gas constant, and equation (11) is used to evaluate  $\langle \tilde{T} \rangle$ , even though temperature is not a dependent variable of equation (1).

The radius of the flame is given by

$$b = \sqrt{\frac{\dot{m}}{\langle \bar{\rho} \rangle \langle \tilde{u} \rangle \pi}}. \quad (15)$$

### 3.2. One-dimensional conservation equations

To obtain the one-dimensional conservation equations, the following procedure is used. First, the general conservation equations for the perturbed and unperturbed flows are subtracted and the result is integrated over a control volume, limited by two cross-sections, infinitely close to each other, and a lateral surface far enough from the center-line, where  $\phi$  tends to  $\phi_a$ . Then, the result is simplified using the parabolic hypothesis and assuming that the difference between the perturbed and unperturbed diffusion fluxes decrease with radial distance faster than  $A^{-1/2}$ ; as a consequence, the diffusion vector vanishes over all the surfaces enclosing the control volume. Finally, the definitions (12) to (15) are applied.

The general equation is

$$\frac{d}{ds} (\dot{m} \langle \tilde{\phi} \rangle) = \phi_a \dot{m}'_0 + \Sigma_\phi, \quad (16)$$

where

$$\dot{m}'_0 = \frac{d\dot{m}_a}{ds} - \lim_{A \rightarrow \infty} \oint_L (\bar{\rho} \tilde{w} - \rho_a v_a \cos \theta) dl \quad (17)$$

is the entrained mass per unit length and time. The argument of the integral in equation (17) tends to zero as  $A^{-1/2}$ ; so that the limit tends to a finite value. The source term in equation (16) is

$$\Sigma_\phi = \lim_{A \rightarrow \infty} \int_A (S_\phi - S_{\phi_a}) dA + \dot{m}_a \frac{d\phi_a}{ds}. \quad (18)$$

### 3.3. Mass entrainment assumptions

To estimate the mass entrainment, two models are used. In the first one,

$$\dot{m}'_0 = 2\pi b \bar{\rho}_a \sqrt{\frac{\langle \bar{\rho} \rangle}{\rho_a}} (\alpha |\langle \bar{u} \rangle - v_a \cos \theta| + \beta |v_a \sin \theta|), \quad (19)$$

where the factor  $(\langle \bar{\rho} \rangle / \rho_a)^{1/2}$  is due to Ricou and Spalding (1961), and  $\alpha$  and  $\beta$  are given the values of 0.057 and 0.5, respectively, in the present model. The second model, due to Tamanini (1981), in which

$$\dot{m}'_0 = C_m \mu_v, \quad (20)$$

is based on the analytical solution for a jet obtained by Schlichting (1968). In UPMFIRE,  $C_m$  is given the value of 20.

The turbulent viscosity is evaluated using the classical k- $\epsilon$  method directly applied to the average values:

$$\langle \mu_t \rangle = C_\mu \langle \bar{\rho} \rangle \frac{\langle k \rangle^2}{\langle \epsilon \rangle}. \quad (21)$$

#### 4. JUMP IN FLOW CONDITIONS ACROSS AN OBSTACLE

The analysis of the interaction of turbulent diffusion flames with an obstacle may be of interest in different scenarios; for example, to estimate the heat transferred to a pipe-line or to a tank in accidental situations.

One-dimensional models are useful to evaluate the interaction with an obstacle whose characteristic length is much smaller than the flame size. We assume that the obstacle is completely engulfed by the flame. The interaction is represented by the drag force,  $D_1$ , and the heat exchanged,  $Q_1$ . Due to the small size of the obstacle, we assume that the problem can still be considered as parabolic, although this assumption fails locally.

To estimate the drag force, we use

$$D_1 = \frac{1}{2} \langle \bar{\rho} \rangle \langle \bar{u} \rangle^2 A_T C_D, \quad (22)$$

where  $A_T$  is the projected area of the obstacle over the plane normal to the center line and  $C_D$  is a drag coefficient, which may depend on the Reynolds number, based on the averaged upstream flow conditions.

The heat exchanged between the flame and the obstacle has two contributions: radiation, which is discussed latter, and convection, calculated using

$$Q_{1c} = \kappa_g (\langle \bar{T} \rangle - T_{ob}) L_{ob} Nu, \quad (23)$$

where  $\kappa_g$  is the gas thermal conductivity,  $T_{ob}$  the obstacle temperature,  $L_{ob}$  the characteristic length of the obstacle, and  $Nu$  the Nusselt number, which depends on the Reynolds number, based on the averaged upstream flow conditions and the Prandtl number.

The jump in flow conditions across the object is represented by source terms in the

conservation equations:

$$\Delta(\dot{m}) = 0 \quad (24)$$

$$\Delta(\dot{m}\langle\tilde{v}_x\rangle) = -D_1\sin\theta \quad (25)$$

$$\Delta(\dot{m}\langle\tilde{v}_z\rangle) = -D_1\cos\theta \quad (26)$$

$$\Delta(\dot{m}\langle\tilde{h}\rangle) = -Q_r \quad (27)$$

$$\Delta(\dot{m}\langle\tilde{\xi}\rangle) = 0 \quad (28)$$

$$\Delta(\dot{m}\langle k\rangle) = -D_1\langle\tilde{u}\rangle \quad (29)$$

$$\Delta(\dot{m}\langle\varepsilon\rangle) = -D_1\langle\tilde{u}\rangle\frac{\langle\varepsilon\rangle}{\langle k\rangle}C_{\varepsilon 1} \quad (30)$$

$$\Delta(\dot{m}\langle g\rangle) = 0 \quad (31)$$

It has been assumed that the energy dissipated by drag is fully converted into turbulent kinetic energy. The classical coefficient of the k- $\varepsilon$ -g model for the production of  $\varepsilon$ ,  $C_{\varepsilon 1}$ , is used. No source term is included in equation (31); although it may be expected that the mixing enhancement due to the obstacle makes g to decrease, this effect is partially taken into account by the increase of  $\varepsilon$ .

## 5. RADIATION TO OBSTACLES ENGULFED BY THE FLAME

To evaluate the heat transferred from the flame to a surface of an engulfed obstacle, the zoning method (Hottel and Sarofim, 1967) is adapted to this case considering an average absorption coefficient for each flame section, so that

$$Q_{ir} = \int_s \int_A \frac{\sigma_b \tilde{T}^4}{\pi} \int_{A_{ob}} \frac{\cos\theta_{ob}}{s^{*2}} \exp\left(-\int_0^{s^*} a ds\right) dA_{ob} dA ds \quad (32)$$

where  $s^*$  is the distance from the flame element to the surface element of the obstacle, and  $\theta_{ob}$  is the angle between the normal to the obstacle and the line joining the flame volume element and the obstacle surface element. The absorption coefficient is estimated by  $a = \log(1-\varepsilon)/(2b)$ . A detailed description can be found in Servert (1993).

## 6. EXPERIMENTAL VALIDATION

The one-dimensional model UPMFIRE has been validated by comparison with both wind-tunnel experiments, carried out by Duijm (1993) and Verheij and Duijm (1991), and full-scale measurements carried out by Ott (1991) and Bennett et al. (1991). A comparison with a three-dimensional model (Hernández and Crespo, 1994) has also been made.

The case of a release of natural gas through a 5 mm nozzle at 250 mm over the ground is first considered. The fuel exit velocity is 12.6 (26.2) m/s in Fig. 1 (2) and the wind speed 1.64 (1.52) m/s at 500 mm over the ground. The ground roughness is  $3.9 \times 10^{-5}$  m. In Figs. 1 and 2, a comparison is shown for the temperature contours in the vertical plane containing the burner axis obtained from the one-dimensional and three-dimensional models (Hernández and Crespo, 1994), and from wind-tunnel experiments (Verheij and Duijm, 1991). The agreement is good, although the temperature contours are in general longer and thinner in the one-dimensional model than in the three-dimensional one.

In Fig. 3, measurements (Ott, 1991) of the thermal radiation flux emitted from the flame to an engulfed vertical cylinder, of a diameter of 0.204 m, are compared with the numerical results obtained from the model, for the case of a release of natural gas through a 50 mm nozzle at 2.5 m over the ground, with a fuel exit velocity of 82.94 m/s. The wind speed is 3.74 m/s at 7 m and 6.59 m/s at 18 m over the ground. The radiation flux has been measured at the horizontal slice, of the cylinder where the flux is maximum, at a height of 2.8 m, and it has been computed for slices at 3.05 m and 2.55 m over the ground, located around the place where the measurements were made. The radiation flux is extremely sensitive to the location of the point of maximum temperature, thus a small error in the flame location leads to very important differences in the calculated heat flux. An interesting conclusion of this work could be that it is convenient to calculate heat flux in a broad area around the points of interest. Taking this sensitivity of the radiative heat flux into account, a good agreement between experiments and model results is found.

Fig. 4 corresponds to an underexpanded release of natural gas through a 75 mm nozzle at 3 m over the ground, with a mass flow rate of fuel of 8 Kg/s, and exit static pressure of 7.52 bar; the conditions where the calculations start are those of the place where ambient pressure is reached, and they have been estimated by using overall conservation equations. The wind speed is 2.3 m/s at 4.1 m over the ground. The obstacle has a diameter of 0.95m, is 15 m downstream from the exit, and its axis is 3 m above the ground. The measurements (Bennett et al., 1991) correspond to a section 0.5 m off the symmetry plane. Calculations correspond to the same position.

In Fig. 5, it is presented a comparison between the calculated and measured values (Ott, 1991) of the radiative heat flux at a surface in the ground looking  $45^\circ$  up to the flame, and at a distance of 2.7 m from the symmetry plane. The agreement is reasonable.

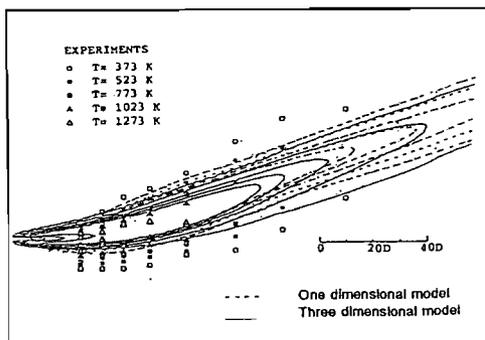


Figure 1. Temperature Contours

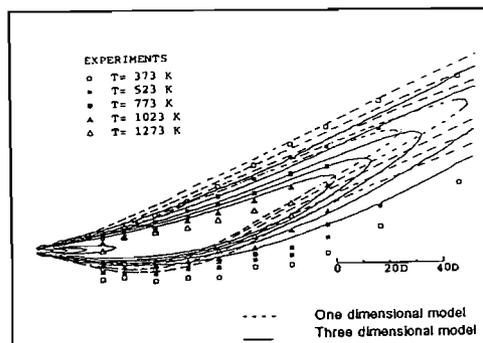


Figure 2. Temperature Contours

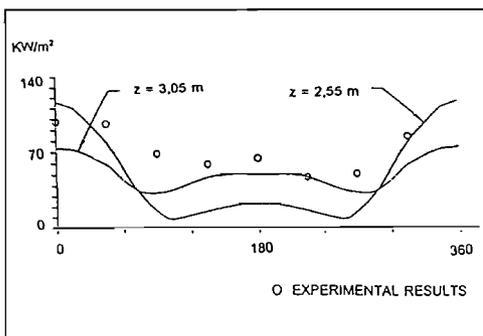


Figure 3. Radiation to a vertical cylinder

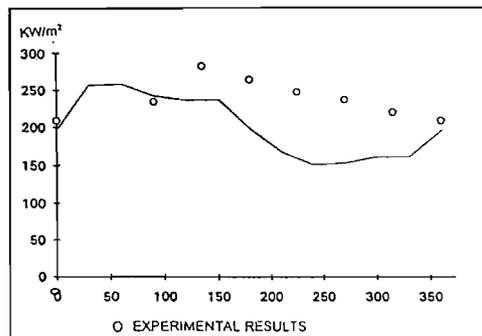


Figure 4. Radiation to a vertical cylinder

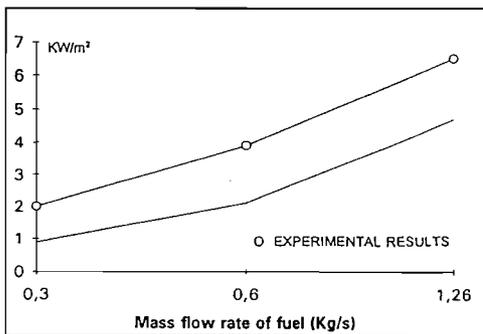


Figure 5. Radiation to a nearby surface

## 7. ACKNOWLEDGEMENTS

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