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PREDICTION OF A TURBULENT REACTING DUCT FLOW WITH SIGNIFICANT RADIATION

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On présente une méthode pour prédire un écoulement turbulent dans un conduit à symétrie axiale où une flamme diffusible se produit, et on développe un modèle pour prédire le rayonnement considérable de chaleur. Ce modèle est incorporé à une procédure disponible pour résoudre le transfert convectif et diffusif de moment, de chaleur, et de masse.

A method is presented for predicting a confined, turbulent, axisymmetrical duct flow in which a diffusion flame occurs. Radiation is important and a model is developed for its prediction which is incorporated into an existing solution procedure for the convective and diffusive transfers of momentum, heat and matter.

1. Introduction

1.1 The problem. In this paper we present a method for predicting the hydrodynamic and thermal behaviour of an axi-symmetrical turbulent diffusion flame confined in a duct (Fig. 1). We suppose that radiation makes a significant contribution to the heat fluxes in the radial direction, but that the axial transfer of heat, by both radiation and conduction, may be neglected. The velocity in the axial direction is supposed everywhere to be of the same sign.

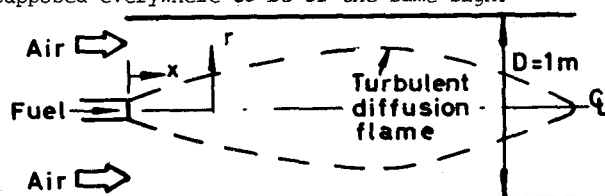


Fig. 1 Geometry and flow conditions of the problem solved

There are some simple industrial flames of this kind; for them the method of prediction will be useful to design engineers. Most industrial flames are however complicated by three-dimensionality and by recirculation of gas flow; for these, a more elaborate prediction procedure is necessary; however, the present treatment of radiation can be extended to these cases, and methods of handling the convective processes either exist or are under development.

1.2 The method of solution. In the absence of radiation, the problem can be solved straightforwardly by application of the finite-difference procedure of Patankar and Spalding [1], which solves coupled non-linear parabolic equations, and which has a built-in model of turbulent transfer.

This method is used in the present work for handling the equations describing the convective and diffusive transfers of momentum, heat and matter; however we have had to extend it so as to account also for the important radiative exchanges. Of course, if the mean free path of radiation were very small in comparison with the flame width, it would be

sufficient to employ the "conduction approximation" of radiation. Usually, however, the flame emissivity is too small to justify this step.

The best-known method of solving the radiative-transfer problems of flames is that of Hottel and Sarofim [2]. This requires the solution of an integro-differential equation, in finite-difference form; the computational task is a heavy one, because each sub-domain of the space influences each other sub-domain, and the influence coefficients are burdensome to compute. We have therefore preferred to employ a formulation introduced by Schuster [3] and elaborated by Hamaker [4], which focusses attention on the fluxes of radiation in two opposed directions, and leads to differential equations which can be solved fairly simply.

Two developments of this latter method have had to be made. First, the equations have required formulation for an axi-symmetrical flow; it emerges that new terms, of non-obvious form, enter to affect appreciably the behaviour. Secondly, it is necessary to express the new equations in a manner which allows their solution, simultaneously with those for velocity, stagnation enthalpy and concentration, by means of the Patankar-Spalding computer program.

In section 2, details of the prediction procedure are given; the greatest attention is devoted to the radiation transfer because of its novelty; the remaining matters are treated fleetingly because of the availability of [1]. Section 3 of the paper is devoted to the description and discussion of the results of particular computations; these have been provided mainly to illustrate the new predictive possibilities, not for comparison with any particular experiments. Such comparisons have not yet been made.

2. General Analysis

2.1 Assumptions. The chemical kinetics are supposed fast enough for the reaction to be physically controlled. The thermodynamics are those of a simple-

chemically reacting system. Three assumptions define this system, they are: that the only reaction is between fuel and oxidant which unite in fixed proportions; that the constant-pressure specific heats of the fuel, oxidant and products are constant and equal; and that the diffusive transport properties: $\Gamma_h, \Gamma_{fu}, \Gamma_{ox}$ and Γ_{prod} are all equal at any point in the fluid. Prandtl's mixing-length hypothesis is employed to determine the effective viscosity of the turbulent flow, and constant turbulent Prandtl/Schmidt numbers are prescribed.

The radiation heat transfer is determined from a two-flux model, these fluxes being opposed and in the radial direction. The angular distribution of both incident and scattered radiation is isotropic. The absorption and scattering coefficients are supposed proportional to the mass concentration of fuel.

2.2 Differential equations. With the preceding assumptions about the chemical kinetics and thermodynamics, three simultaneous conservation equations for momentum, enthalpy and mixture fraction enable the convective heat and mass transfer and combustion to be determined. These equations are:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \mu_{eff} \frac{\partial u}{\partial r}) - \frac{dp}{dx}, \quad (1)$$

$$\rho u \frac{\partial h}{\partial x} + \rho v \frac{\partial h}{\partial r} = -\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff} \frac{\partial h}{\partial r}) + \frac{1}{r} \frac{d(rQ)}{dr}, \quad (2)$$

$$\rho u \frac{\partial f}{\partial x} + \rho v \frac{\partial f}{\partial r} = -\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff} \frac{\partial f}{\partial r}). \quad (3)$$

One further differential equation is required to predict the radiation transfer; this equation is now derived.

Consider an annular ring of thickness dr , at a distance r from an axis of symmetry in an absorbing and scattering medium (see Fig. 2). Let the radiation flux travelling in the direction of positive r be designated by I ; and that travelling in the direction of negative r by J . Let the absorption and scattering coefficients of the medium have the symbols a and s , respectively.

Consider the radiation energy flow $2\pi r I$ traversing the thickness dr of the annular ring. A fraction $2\pi r a dr$ is absorbed; and, if the scattering is isotropic, a fraction $2\pi r \frac{s}{2} I dr$ is eliminated by backward scattering in the direction of negative r . The energy flow $2\pi r I$ is augmented by a fraction $2\pi r \frac{s}{2} J dr$ due to backward scattering of the J flux. If the incident radiation is isotropic, it is further augmented by a fraction $\frac{dr}{r}$ of the flux which enters the ring of radius $r + dr$, but which does not leave the ring of

radius r . Finally, it is augmented by a fraction $2\pi r a E dr$ due to emission from the gases and particles within the ring.

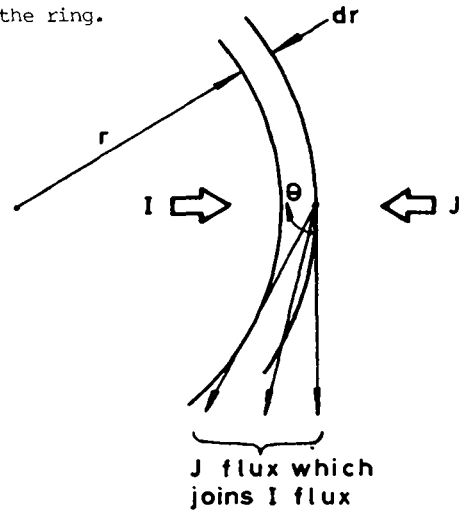


Fig. 2. Sketch showing radiation fluxes

Summation of all of these influences on the flow $2\pi r I$ yields a differential equation for the variation of the flux I with radius, namely:

$$\frac{d(rI)}{dr} = r[-(a+\frac{s}{2}) I + \frac{s}{2} J + \frac{J}{r} + aE]. \quad (4)$$

The coefficient a which multiplies E can be verified as the correct one by consideration of the case of thermal equilibrium where $I = J = E$ and $d(rI)/dr = J/r$. The variation of the J flux can be deduced from analogous arguments; the result is:

$$\frac{d(rJ)}{dr} = r[(a+\frac{s}{2}) J - \frac{s}{2} I + \frac{J}{r} - aE]. \quad (5)$$

Equation 4 and 5 are the foundation on which our theory rests. It is the terms J/r , and the presence of r to the right of the differentiation sign, that distinguish them from those of [2,3]. The two equations can be combined to yield a second order differential equation:

$$\frac{d}{dr} \left(\frac{r^2}{1+(a+s)r} \frac{dF}{dr} \right) + ar(E - F) = 0, \quad (6)$$

where F stands for the quantity $(I+J)$. This is the equation describing the radiation transfer which we solve simultaneously with equations 1 to 3. The radiation heat flux $Q = I - J$ is calculable from the relation:

$$Q = \frac{2r}{1+(a+s)r} \frac{dF}{dr} \quad (7)$$

2.3 The solution procedure. The computer-based solution procedure of Patankar and Spalding is described in detail in [1]. It solves parabolic equations of the form:

$$\frac{\partial \phi}{\partial x} + (a + b_{ij}) \frac{\partial \phi}{\partial w} = \frac{\partial}{\partial w} \left(c \frac{\partial \phi}{\partial w} \right) + d_{\phi}, \quad (8)$$

where ϕ stands for a dependent variable;

$w \equiv (\psi - \psi_I) / (\psi_E - \psi_I)$ is a dimensionless stream function;

$\psi \equiv$ stream function which ranges from ψ_I to ψ_E ;

$a \equiv -(d\psi_I/dx) / (\psi_E - \psi_I)$; $b \equiv -(d(\psi_E - \psi_I)/dx) / (\psi_E - \psi_I)$;

$c_\phi \equiv r^2 \rho u \mu_{eff} / [(\psi_E - \psi_I)^2 \sigma_{eff}]$

and d_ϕ is a source term.

Couette-flow formulae are incorporated which determine the fluxes of heat, mass and momentum near walls. Marching integration is employed, iteration being entirely avoided. The procedure permits a set of simultaneous equations which possess the common form of 8 to be solved very rapidly.

Equations 1, 2, 3 and 6 all possess the form of equation 8, with ϕ standing respectively for u , h , f and F ; but convection terms, represented by those on the left-hand side of equation 8, are absent from equation 6. This difference is, however, easily resolved by multiplying the terms on the right-hand side of equation 8, when ϕ stands for F , by a factor sufficiently large to make negligible the influence of those to the left of the equal sign.

The Patankar-Spalding solution procedure permits

linearization of the source term over the forward step. We have availed of this feature in the case of equation 6 and have expressed its source term, the second one, as:

$$d_F = \frac{a}{\rho u} (E_U - F_D) \tag{9}$$

where the subscripts U and D refer to the upstream and downstream locations between which a forward step is made. The source term of equation 2,

$d_h = \frac{1}{\rho u r} \frac{d(rQ)}{dr}$, is not linearized and is expressed from equations 6 and 7 as:

$$d_h = - \frac{2a}{\rho u} (E_U - F_U) \tag{10}$$

These formulations for the source terms ensure a correct enthalpy balance and result in good computational stability.

The radiation flux streaming from a wall is the summation of the reflected incident flux plus the wall emission:

$$J_w = (1 - \epsilon_w) I_w + \epsilon_w E_w \tag{11}$$

Using equation 7 and the definitions of F and Q , this relation can be recast as:

$$\left[\frac{r}{1+(a+s)r} \frac{dF}{dr} + \frac{\epsilon}{2-\epsilon} (F - E) \right]_w = 0 \tag{12}$$

This is the boundary condition which must be applied

to equation 6 at the duct wall. It is unusual in that both the gradient and magnitude of the dependent variable F are prescribed. We have incorporated it into the finite-difference scheme of the solution procedure using an implicit formulation.

3. Particular Computations

3.1 Problem specification. The duct of Fig. 1 is 1 m in diameter and is cooled to a uniform temperature of 363°K. The fuel is oil and the firing rate is 3.1×10^7 W. The air is at ambient conditions and its flow rate is 20% in excess of the stoichiometric requirements. The density of the gaseous mixture is calculated from the equation of state; its laminar viscosity is presumed to vary as the temperature raised to the power one half. The mixing length varies in accordance with following specification:

$$0.4y \ll \lambda D / 2\kappa, \quad \ell = \kappa y \{ 1 - \exp[-\sqrt{17} \rho / (27\mu)] \} ; \tag{13a}$$

$$\lambda D / 2\kappa \ll y \ll D / 2, \quad \ell = \lambda D / 2; \tag{13b}$$

where y is the distance from the wall and κ and λ are constants assigned the values 0.44 and 0.09 respectively. The turbulent Prandtl/Schmidt numbers are equal to 0.86.

It is not the intention here to suppose formulae for absorption and scattering coefficients in keeping

with the most recent knowledge. An adequate demonstration of the capabilities of the flux-model can be effected using very simple formulae which nevertheless are not wholly unrealistic. In this spirit, we presume that the absorption and scattering coefficients are proportional to the mass concentration of fuel, hence:

$$a = \gamma_a m_{fu}, \tag{14a}$$

$$\text{and } s = \gamma_s m_{fu}, \tag{14b}$$

where the γ 's are the constants of proportionality.

3.2 Some results Fig. 3 shows the distribution of wall heat flux over a length of 10 duct diameters downstream of the fuel injection location. Curves are shown for values of γ_a ranging from 2 to 40 in the absence of scattering. The maximum value of the absorption coefficient space-averaged across the duct \bar{a}_{max} is indicated for each value of γ_a . These vary from 0.14 to 2.8, a range which includes values typically encountered in oil-fired furnaces. The shapes of the heat-flux distributions are also typical of those measured in furnace trials. The maximum heat flux occurs at an x/D of about 1.7 in each case. The ratio of the maximum to averaged heat fluxes increases with increasing absorption.

The increase in the heat flux relative to an increase in γ_a becomes progressively less since the absorptivity cannot exceed unity. Although not shown on Fig. 3, the convective wall heat transfer is also an outcome of the solution. When δ_a is 40, for example, it rises slowly with x reaching the significant value of $5.7 \times 10^4 \text{ W/m}^2$ at $x/D = 10$.

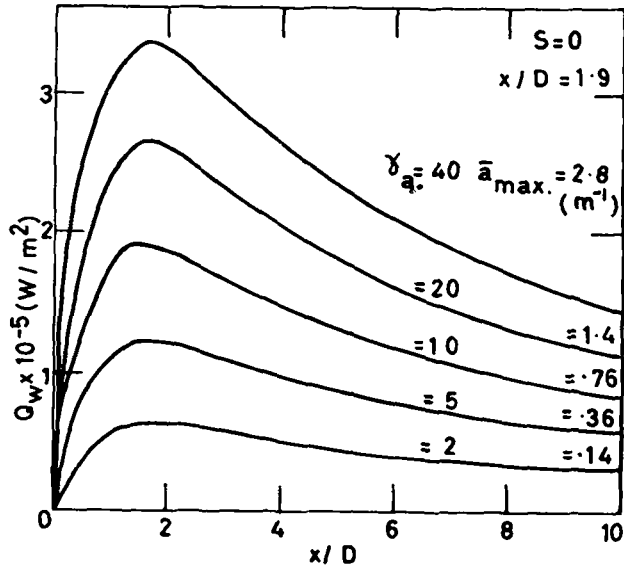


Fig. 3. Distribution of wall heat flux

Fig. 4 exhibits temperature profiles at two downstream stations: $x/D = 1.9$ and 8.2 . Profiles are shown at both stations for two cases: without radiation transfer, and with radiation corresponding to $\gamma_a = 40$ and no scattering. This amount of radiation lowers the maximum temperatures, which of course occur at the flame location, by about 260°C at $x/D = 1.9$ and by about 420°C at $x/D = 8.2$. The maximum temperatures are still higher than would occur in practice, they exceed the adiabatic flame temperature, but a more judicious specification of specific heat would correct this. The decrease in flame temperature caused by radiation has the consequence of diminishing the importance of dissociation which cannot be properly accounted for by simple theoretical models of chemical reaction. Note that the radiation removes heat from the central region of the flow with the result that the temperature rise there due to conduction from the flame between the two stations is only small.

Fig. 5 displays profiles of heat flux at the station $x/D = 1.9$ for γ_a ranging from 2 to 40 and no scattering. The profiles have the expected shapes. They are included because they demonstrate that local information about the heat flux can readily be obtained using the present procedure. Such information is of great value when the location of,

say, a superheater in a boiler is to be determined.

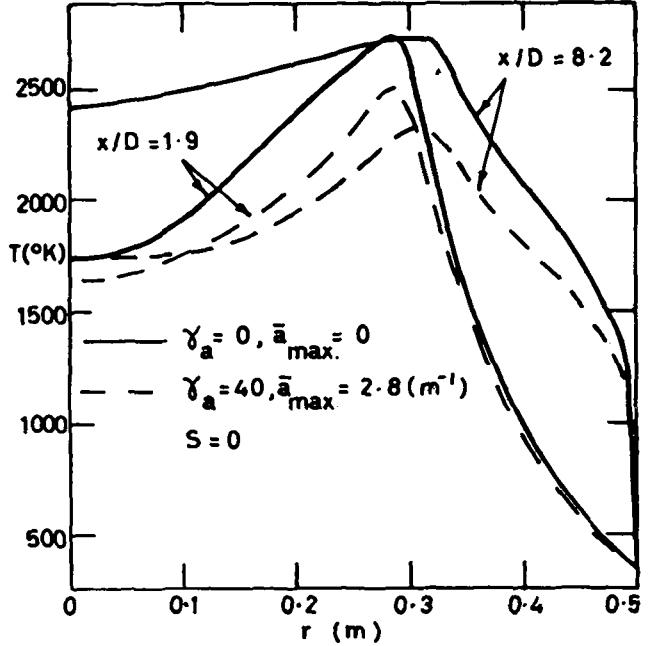


Fig. 4: Temperature profiles

The soot particles formed in oil flames are small enough for scattering to be negligible. The particles may, however, agglomerate; and cenospheres may be present. Also, the particles in a pulverized-coal flame are not small enough for scattering to be insignificant. The complete radiation theory must, therefore, be capable of handling scattering. In Fig. 6 two heat-flux profiles are presented for $\delta_a = 40$ at $x/D = 1.9$; the broken curve is obtained

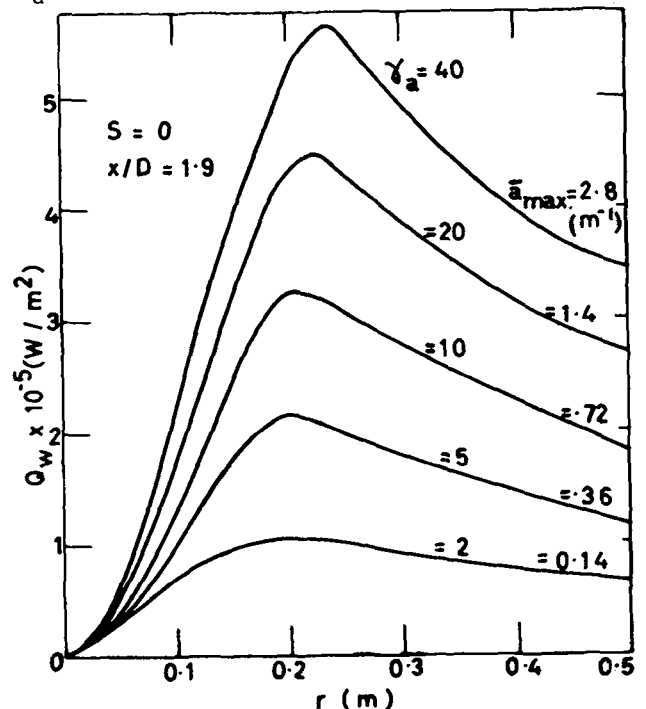


Fig. 5 Heat-flux profiles

when there is no scattering, while the solid curve is the result when the ratio of scattered to absorbed radiation is one half. The effect of this rather large amount of scatter is negligible. This was also found to be the case for smaller values of γ_a . Of course, scattering is not, in general, isotropic as assumed in the present analysis. This assumption is, however, not a requirement of the flux model.

5. Conclusions

A numerical method has been presented which enables the entire hydrodynamic and thermal nature of a chemically-reacting, absorbing and scattering flow to be predicted. The feasibility of the method has been demonstrated through its application to the prediction of a turbulent duct flow containing a diffusion flame. The method is rapid. Using 20 grid divisions in the radial direction and with a forward step size equal to 1/50 of the duct radius, the time required by an IBM 7094 to compute solutions in the range $0 \leq x/D \leq 10$ was typically 2 minutes. The development of the method is, however, in its early stages. Intensive testing is yet required before the status of a reliable design tool for the practising engineer can be accorded to it.

6. Nomenclature

- a · scattering coefficient
- \bar{a}_{max} maximum value of a space-averaged across duct
- D duct diameter
- E emissive power
- f mixture fraction defined as mass of fuel-bearing stream which has mixed with oxidant-bearing stream to produce unit mass of products.
- F (I+J), the sum of the radiation fluxes
- h specific enthalpy
- m mass fraction
- p pressure
- r radial distance
- s scattering coefficient

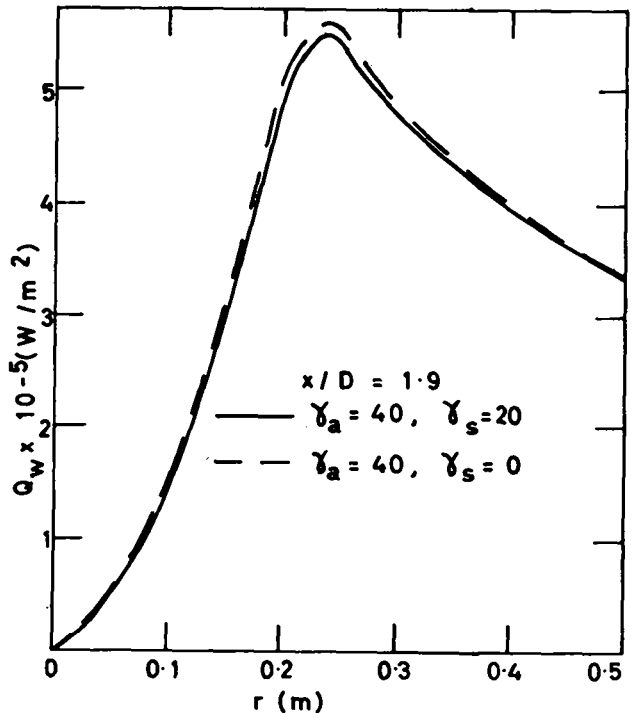


Fig. 6: Effect of scattering

- u streamwise velocity
- v radial velocity
- x streamwise distance from fuel-injection station
- y distance from and normal to the duct wall
- Γ μ/σ , a diffusive transport coefficient
- γ_a a/m_{fu} , an absorption constant
- γ_s s/m_{fu} , a scattering constant
- ϵ emissivity
- χ a mixing-length constant
- λ a mixing-length constant
- μ fluid viscosity
- ρ fluid density
- σ Prandtl/Schmidt number
- δ a dependent variable

Subscripts

- eff effective sum of laminar and turbulent contributions
- fu, ox, prod fuel, oxidant, products
- w wall value

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