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On Diffusion Flames in Turbulent Shear Flows: Modeling Reactant Consumption in a Circular Fuel Jet

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The turbulent portion of the circular fuel jet is analyzed for isobaric subsonic flow under fast direct one-step irreversible reaction between unpremixed fuel and oxidant. Mean spatial profiles for the dependent variables are found numerically from the governing nonlinear partial differential equations, based upon an explicit eddy diffusion and upon a mean rate of reactant consumption proportional to the product of the mean mass fraction of fuel, the mean mass fraction of oxidant, and the appropriate local characterization of the mean rate of strain. Experimental results are employed to evaluate the pertinent constants in the theoretical formulation of the model.

I. Introduction

THE structure of the turbulent diffusion flame in the *circular* fuel-jet geometry is studied theoretically. As such, this represents an extension of the work by Bush, Feldman, and Fendell on the structure of turbulent diffusion flames in the *planar* fuel-jet[1] and in the planar mixing-layer[2] geometries. In this present paper, as in these previous papers, the emphasis is on the solution of a model formulation of the boundary-value problem for a turbulent diffusion flame in a flow geometry of practical interest, when the model is based upon the premise that the consumption of reactants and the generation of product(s) and chemical exothermicity are controlled by unsteady, inviscid, inertial, large-scale mixing.

In this model, in time-average, for a direct one-step irreversible bimolecular chemical reaction, the mean rate of reactant consumption is taken to be related to the product of the mean mass fraction of oxidant, the mean mass fraction of fuel, and the magnitude of the principal mean strain rate (for the parabolic formulation appropriate for the thin shear layers of interest here). It is argued (as in Refs. 1 and 2) that, in general, the magnitude of the principal mean strain rate furnishes a characteristic frequency for the mean rate of local chemical activity in a turbulent diffusion flame in which macroscopic mixing is rate-controlling. This explicit local algebraic (as opposed to field-type differential) expression adopted for the mean rate of chemical reaction is compatible with the adoption of an explicit local algebraic (eddy viscosity) expression for the mean rate of diffusive transport.

The present model was first studied in detail for the planar mixing layer formed by two parallel streams.[2] However, whereas the fully developed mixing layer is tractable for analysts, it is not tractable for experimentalists and, therefore, some empirical constants in the theory remained unassigned for lack of data. Experimentalists[3-8] have treated the fuel jet exhausting into an oxidant-containing ambient, and, under the assumption that values for empirical factors may be transferable between geometries, solutions were determined for the planar fuel jet.[1] Unfortunately, the only data on planar turbulent free-jet diffusion flames (known to the authors) were the limited measurements due to Kremer.[9] Thus, it was necessary to consider experimental results for axisymmetric turbulent free-jet diffusion flames for purposes of qualitative comparison, let alone quantitative comparison. Here, for direct comparison with these axisymmetric experimental results, axisymmetric theoretical results are obtained.

The formulation of the high-Reynolds-number, low-Mach-number boundary-value problem for the circular fuel jet is presented, based upon the previously mentioned model for the mean rate of reactant consumption when macroscopic mixing is rate-controlling. (See Ref. 1 for the planar fuel-jet formulation of this particular model boundary-value problem.) A modified Howarth transformation is introduced to produce an "incompressible" formulation of the boundary-value problem (see Ref. 1 for the planar transformation and Ref. 10 for the axisymmetric transformation). Also introduced are the "incompressible" (turbulent) Shvab-Zeldovich functions, linear sums of the dependent variables mean temperature and the species (stoichiometrically adjusted) mean mass fractions.

First, the self-similar closed-form solutions for the mean velocity field and the mean (modified) mass-fraction Shvab-Zeldovich function are developed (see Refs. 1 and 10 for the planar and axisymmetric cases, respectively). For these solutions, it is taken that the transformed eddy viscosity is a constant. Experimental results[4,7] are employed to evaluate the constants of integration in these solutions. In turn, based upon these similarity solutions, the model boundary-value problem is developed for the determination of the mean (stoichiometrically-adjusted) mass fraction of fuel in the region downstream of the "effective" jet exit. The dependence of the solution of this model boundary-value problem for the fuel mass-fraction function on the product of the two empirically determined parameters: the jet growth rate γ'' and the (constant) effective Damköhler number B'' is shown.

Numerical solutions of this circular-fuel-jet boundary-value problem are obtained by the method of Sincovec and Madsen.[11] For the assignment of parameters for this problem, the case chosen for numerical study is that of a turbulent jet of pure carbon monoxide gas at room temperature exhausting into stagnant air. The previously obtained selfsimilar results for the axial velocity and the mass-fraction Shvab-Zeldovich function are presented and compared with experimental results obtained for these flow quantities. From these comparisons, a value of γ'' for the

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chemically reacting circular-jet flow geometry is obtained. From a preliminary parametric study, with respect to $(\gamma''B'')$, of the numerical solutions, the value of $(\gamma''B'')$ that produces the experimentally observed value of the temperature at the flame tip is determined.

In addition to numerical solutions for the fuel and oxidant mass-fraction and temperature profiles, for the parameters of the carbon monoxide circular fuel jet, and for the prescribed values of γ'' and $(\gamma''B'')$, those for the flame and maximum temperature loci are presented.

II. Formulation

The direct one-step irreversible bimolecular chemical reaction

$$F+O\rightarrow P \tag{1}$$

in which fuel F and oxidant O yield product P is considered. The steady-state flow geometry studied is that of a low-speed circular fuel jet exhausting into a stagnant atmosphere containing oxidant. In the limit of $R=\rho_r u_r \ell_r/\mu_r$, the (reference) Reynolds number, going to infinity and $M=u_r/(\gamma RT_r)^{1/2}$, the (reference) Mach number, going to zero, the (nondimensional) boundary-layer approximations to the governing conservation equations for the time-averaged description of the turbulent reacting jet are[1,10]:

$$\frac{\partial(\rho u)}{\partial x}+\frac{1}{r}\frac{\partial(r\rho v)}{\partial r}=0 \tag{2}$$

$$\rho\left(u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial r}\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\epsilon\frac{\partial u}{\partial r}\right) \tag{3}$$

$$\rho\left(u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial r}\right)=\frac{1}{\sigma_h}\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\epsilon\frac{\partial T}{\partial r}\right)+Q\dot{w} \tag{4}$$

$$\rho\left(u\frac{\partial Y_i}{\partial x}+v\frac{\partial Y_i}{\partial r}\right)=\frac{1}{\sigma_i}\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\epsilon\frac{\partial Y_i}{\partial r}\right)+\dot{w}_i$$

with

$$i=F,O,P \tag{5}$$

Here: $x=x_k/\ell_r$ and $r=r_k/\ell_r$ are the streamwise and normal spatial coordinates, respectively, with $0\le x<\infty$, $0\le r<\infty$, with ℓ_r = reference length (the initial jet diameter); $u=u_k/u_r$ and $v=v_k/u_r$ are the mean streamwise and normal velocity components, respectively, with u_r = reference velocity (the initial jet velocity); $\rho=\rho_k/\rho_r$ and $T=T_k/T_r$ are the mean density and (absolute) temperature of the mixture, respectively, with $\rho_r RT_r=p_r$, where p_r = reference pressure (the background and jet pressure); Y_i is the mean (stoichiometrically adjusted) mass fraction of species i; $Q=Q_k/c_pT_r$ is the specific heat of combustion, while $\dot{w}(=-\dot{w}_F=-\dot{w}_O=\dot{w}_P)=\dot{w}_k/(\rho_r u_r/\ell_r)$ is the mean rate of reactant consumption (and product generation); $\epsilon=\epsilon_k/u_r\ell_r$ is the eddy viscosity (or turbulent momentum-diffusion coefficient), while σ_h and σ_i are the (constant) turbulent Prandtl number and turbulent Schmidt number for species i, respectively, such that ϵ/σ_h and ϵ/σ_i are the turbulent heat-conduction and species-diffusion coefficients. Further, the (nondimensional) equation of state is postulated to be:

$$p=\rho T=1 \tag{6}$$

where $p=p_k/p_r$ is the mean pressure, and the molecular weights of all species present are taken as comparable. The mean reaction rate is postulated to be[1,2]:

$$\dot{w}=\left(\rho\beta\left|\frac{\partial u}{\partial r}\right|\right)Y_FY_O \tag{7}$$

where β is the (nondimensional) function that characterizes the rate of chemical consumption relative to the rate of species transport. For this system of equations, it is taken that stagnant uniform conditions characterize the ambient, specifically:

$$u\rightarrow u_\infty=0,\ T\rightarrow T_\infty=1$$

$$Y_F\rightarrow Y_{F\infty}=0,\ Y_O\rightarrow Y_{O\infty}=\text{const}$$

$$\text{as } r\rightarrow\infty \tag{8}$$

At the centerline, it is taken that

$$v,\frac{\partial u}{\partial r},\frac{\partial T}{\partial r},\frac{\partial Y_F}{\partial r},\frac{\partial Y_O}{\partial r}\rightarrow 0 \quad \text{as } r\rightarrow 0 \tag{9}$$

The initial conditions at the jet exit plane are

$$u\rightarrow u_j=1,\ T\rightarrow T_j=\text{const}$$

$$Y_F\rightarrow Y_{Fj}=\text{const},\ Y_O\rightarrow Y_{Oj}=0 \quad \text{for } 0\le r<1/2$$

$$\text{as } x\rightarrow x_j=0 \tag{10a}$$

$$u\rightarrow u_\infty=0,\ T\rightarrow T_\infty=1$$

$$Y_F\rightarrow Y_{F\infty}=0,\ Y_O\rightarrow Y_{O\infty}=\text{const} \quad \text{for } 1/2<r<\infty$$

$$\text{as } x\rightarrow x_j=0 \tag{10b}$$

The specified functions of Eqs. (10) are compatible with Eqs. (8), and with the requisite of initially unmixed reactants.

For $R\rightarrow\infty$, $M\rightarrow 0$, and $p=1$, with the introduction of the coordinate transformation

$$(x,r)\rightarrow(x,z),\ \text{with } z=\left[2\int_0^r \rho r'\,dr'\right]^{1/2} \tag{11a}$$

and of the velocity transformation

$$(u,v)\rightarrow(U,V),\ \text{with } U=u,\ V=u\frac{\partial z}{\partial x}+v\frac{\partial z}{\partial r} \tag{11b}$$

Equations (2-7) may be re-expressed as

$$\frac{\partial U}{\partial x}+\frac{1}{z}\frac{\partial(zV)}{\partial z}=0\text{: } U=\frac{1}{z}\frac{\partial\Psi}{\partial z},\ V=-\frac{1}{z}\frac{\partial\Psi}{\partial x} \tag{12}$$

$$U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial z}-\frac{1}{z}\frac{\partial}{\partial z}\left(zD''\frac{\partial U}{\partial z}\right)=0 \tag{13}$$

$$U\frac{\partial T}{\partial x}+V\frac{\partial T}{\partial z}-\frac{1}{\sigma_h}\frac{1}{z}\frac{\partial}{\partial z}\left(zD''\frac{\partial T}{\partial z}\right)$$
$$=Q\left(B''\left|\frac{\partial U}{\partial z}\right|\right)Y_FY_O \tag{14}$$

$$U\frac{\partial Y_i}{\partial x}+V\frac{\partial Y_i}{\partial z}-\frac{1}{\sigma_i}\frac{1}{z}\frac{\partial}{\partial z}\left(zD''\frac{\partial Y_i}{\partial z}\right)$$
$$=-\left(B''\left|\frac{\partial U}{\partial z}\right|\right)Y_FY_O,\ \text{with } i=F,O \tag{15}$$

In the above equations,

$$D''=\frac{r^2\rho^2}{\left[2\int_0^r \rho r' \mathrm{d}r'\right]}\epsilon \tag{16a}$$

$$B''=\frac{r\rho}{\left[2\int_0^r \rho r' \mathrm{d}r'\right]^{1/2}}\beta \tag{16b}$$

Further, Eqs. (8-10) may be re-expressed as:

$$U\to U_\infty=0,\ T\to T_\infty=1$$
$$Y_F\to Y_{F\infty}=0,\ Y_O\to Y_{O\infty}=\text{const}$$
$$\text{as } z\to\infty \tag{17}$$

$$V,\frac{\partial U}{\partial z},\frac{\partial T}{\partial z},\frac{\partial Y_F}{\partial z},\frac{\partial Y_O}{\partial z}\to 0$$
$$\text{as } z\to 0 \tag{18}$$

$$U\to U_j=1,\ T\to T_j=\text{const}$$
$$Y_F\to Y_{Fj}=\text{const},\ Y_O\to Y_{Oj}=0 \quad \text{for } 0\le z<z_j$$
$$\text{as } x\to x_j=0 \tag{19a}$$

$$U\to U_\infty=0,\ T\to T_\infty=1$$
$$Y_F\to Y_{F\infty}=0,\ Y_O\to Y_{O\infty}=\text{const} \quad \text{for } z_j<z<\infty$$
$$\text{as } x\to x_j=0 \tag{19b}$$

Under the transformation of Eq. (11a), $z\to z_j=(1/4T_j)^{1/2}$ as $r\to 1/2$.

Since, experimentally σ_h, $\sigma_i\simeq\sigma$, it is convenient to introduce the (turbulent) Shvab-Zeldovich functions Φ_q, linear sums of the dependent variables T and Y_i. The functions adopted here are:

$$\Phi_Y=(Y_F-Y_O)\equiv Y$$
$$\Phi_T=T+{1/2}Q(Y_F+Y_O)\equiv\Theta \tag{20}$$

From Eqs. (14) and (15), it is found that the conservation equations for these Shvab-Zeldovich functions are:

$$U\frac{\partial\Phi_q}{\partial x}+V\frac{\partial\Phi_q}{\partial z}-\frac{1}{\sigma}\frac{1}{z}\frac{\partial}{\partial z}\left(zD''\frac{\partial\Phi_q}{\partial z}\right)=0 \tag{21}$$

From an analysis based upon Eqs. (19-21) and parallel to the one presented in Ref. 1, the following expression for T as a function of Y_F and Y_O is obtained:

$$T=1+\frac{(T_j-1)(Y_F+(Y_{O\infty}-Y_O))}{(Y_{Fj}+Y_{O\infty})}+\frac{QY_{Fj}Y_{O\infty}}{(Y_{Fj}+Y_{O\infty})}\left(1-\frac{Y_F}{Y_{Fj}}-\frac{Y_O}{Y_{O\infty}}\right) \tag{22}$$

III. Analysis

With D'' a specified spatial function, at most, the mean velocity-field initial/boundary-value problem for the jet geometry is governed by Eqs. (12) and (13) and the *pertinent* boundary/initial conditions of Eqs. (17-19). Integration of the momentum equation, Eq. (13), subject to the initial conditions of Eq. (19), yields the momentum flux K'', an integral flow quantity, defined by

$$K''=2\pi\int_0^\infty U^2 z\mathrm{d}z=\pi z_j^2=\frac{\pi}{4T_j} \tag{23}$$

With the introduction of the "effective jet exit" plane $x_i(>0)$, of the "normal length" function $z_*(x)=z_i(x/x_i)$ with $z_i=\text{const}$, of the "centerline velocity" function $U_*(x)=u_i(x/x_i)^{-1}$ with $u_i=\text{const}$, and of the coordinates

$$\xi=(x/x_i),\ \eta=(z/z_*(x))=\gamma''(z/x) \tag{24a}$$

where $\gamma''=(x_i/z_i)=$(constant) spreading parameter (to be determined empirically), and with the introduction of the stream function

$$\Psi(x,z)=\Psi(\xi,\eta)=U_*(\xi)z_*^2(\xi)F(\eta)=(u_iz_i^2)\xi F(\eta) \tag{24b}$$

the velocity components and the vorticity (in the domain $0\le\eta<\infty$, $1\le\xi<\infty$) can be written as

$$U=\frac{1}{z}\frac{\partial\Psi}{\partial z}=\frac{u_i}{\xi}\left[\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right]$$
$$V=-\frac{1}{z}\frac{\partial\Psi}{\partial x}=\frac{1}{\gamma''}\frac{u_i}{\xi}\left[\frac{\mathrm{d}F}{\mathrm{d}\eta}-\frac{F}{\eta}\right] \tag{25a}$$

$$\frac{\partial U}{\partial z}=\frac{\partial}{\partial z}\left(\frac{1}{z}\frac{\partial\Psi}{\partial z}\right)=\frac{(u_i/z_i)}{\xi^2}\left[\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)\right] \tag{25b}$$

Thus, the boundary conditions of Eqs. (17) and (18) can be written as

$$\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\to 0 \text{ as } \eta\to\infty,$$
$$\left(\frac{\mathrm{d}F}{\mathrm{d}\eta}-\frac{F}{\eta}\right),\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)\to 0 \text{ as } \eta\to 0 \tag{26a}$$

while, by definition,

$$\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\to 1 \text{ as } \eta\to 0 \tag{26b}$$

For the explicit eddy viscosity formulation for D'',

$$D''(x,z)=D''(\xi)=\frac{1}{2\gamma''}U_*(\xi)z_*(\xi)$$
$$=D''=\frac{1}{2\gamma''}(u_iz_i)=\text{const} \tag{27}$$

it can be shown that, for the dynamics, the problem reduces to the following self-similar form:

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\eta\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)+2\frac{F}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)=0\ (0\le\eta<\infty) \tag{28a}$$

$$\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\to 0 \text{ as } \eta\to\infty$$

$$F, \frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)\to 0, \ \frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\to 1 \text{ as } \eta\to 0 \tag{28b}$$

Successive integrations of Eq. (28a), with application of the boundary conditions of Eq. (28b), yield the solution

$$F(\eta)=\left[\frac{\eta^2}{2(1+\frac{1}{4}\eta^2)}\right] \tag{29}$$

Based upon this solution, it is determined that

$$K''=2\pi(u_iz_i)^2\int_0^\infty\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)^2\eta\mathrm{d}\eta=\frac{4\pi}{3}(u_iz_i)^2=\frac{\pi}{4T_j} \tag{30}$$

Thus, $u_iz_i=u_i(x_i/\gamma'')=(3/16T_j)^{1/2}$. If it is taken that $U(\xi,0)=1$ for $0\le\xi\le1$,[7] then it is consistent to take $u_i=1$. For $u_i=1$, from the above, it follows that $z_i=(x_i/\gamma'')=(3/16T_j)^{1/2}$.

Based upon the preceding, the solutions for Ψ, U, V, and $|\partial U/\partial z|$, for $u_i=1$, $z_i=(x_i/\gamma'')=(3/16T_j)^{1/2}$, in the domain $(1\le\xi<\infty, 0\le\eta<\infty)$, are taken to be

$$\Psi=\left(\frac{3}{16T_j}\right)\xi\left[\frac{\eta^2}{2(1+\frac{1}{4}\eta^2}\right] \tag{31a}$$

$$U=\frac{1}{\xi}\left[\frac{1}{(1+\frac{1}{4}\eta^2)^2}\right],\ V=\frac{1}{\gamma''\xi}\left[\frac{\eta(1-\frac{1}{4}\eta^2)}{2(1+\frac{1}{4}\eta^2)^3}\right] \tag{31b}$$

$$\left|\frac{\partial U}{\partial z}\right|=\left(\frac{16T_j}{3}\right)^{1/2}\frac{1}{\xi^2}\left[\frac{\eta}{(1+\frac{1}{4}\eta^2)^3}\right] \tag{31c}$$

The solution given in Eq. (31a) is recognized as a modified form of Schlichting's solution for the incompressible circular jet (see Ref. 10). For the record, the eddy-viscosity parameter of Eq. (27) is given by $D''=(3/64T_j)^{1/2}(1/\gamma'')$.

With $\sigma_i\simeq\sigma$, the initial/boundary-value problem for the (modified) Shvab-Zeldovich function $\bar{Y}=(Y_F+(Y_{O\infty}-Y_O))/(Y_{Fj}+Y_{O\infty})$ for the jet geometry is governed by Eq. (21) and the *pertinent* boundary/intitial conditions of Eqs. (17-19). The species flux integral associated with this function is

$$N''=2\pi\int_0^\infty U\bar{Y}z\mathrm{d}z=\pi z_j^2=\frac{\pi}{4T_j}=K'' \tag{32}$$

In light of the approximations already adopted for the velocity field (see Eq. (31)), it is taken that $\bar{Y}$ is of the form

$$\bar{Y}(x,z)=\bar{Y}(\xi,\eta)=\bar{Y}_*(\xi)G(\eta)=(C_i/\xi)G(\eta) \tag{33}$$

With the introduction of this form for $\bar{Y}$, the above-mentioned forms for Ψ and its derivatives, etc., the problem for this Shvab-Zeldovich function reduces to

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\eta\frac{\mathrm{d}G}{\mathrm{d}\eta}+2\sigma FG\right)=0\ (0\le\eta<\infty),$$

$$G\to0 \text{ as } \eta\to\infty \tag{34a}$$

$$\frac{\mathrm{d}G}{\mathrm{d}\eta}\to0,\quad G\to1 \text{ as } \eta\to0 \tag{34b}$$

Integration of Eq. (34a), subject to the boundary conditions of Eq. (34b), yields the solution

$$G(\eta)=\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)^\sigma=\left[\frac{1}{(1+\frac{1}{4}\eta^2)^{2\sigma}}\right] \tag{35}$$

Based upon this solution, the species flux integral N'', for $u_i=1$, $z_i=(x_i/\gamma'')=(3/16T_j)^{1/2}$, is given by

$$N''=\frac{\pi}{4T_j}\left[\frac{3}{2}C_i\int_0^\infty\left(\frac{1}{\eta}\frac{\mathrm{d}F}{\mathrm{d}\eta}\right)G\eta\mathrm{d}\eta\right]$$
$$=\frac{\pi}{4T_j}\left[\left(\frac{3}{1+2\sigma}\right)C_i\right]=\frac{\pi}{4T_j} \tag{36}$$

Thus, $C_i=((1+2\sigma)/3)$.

Therefore, the solution for $\bar{Y}$, for $u_i=1$, $z_i=(x_i/\gamma'')=(3/16T_j)^{1/2}$, $C_i=((1+2\sigma)/3)$, in the domain $(1\le\xi<\infty, 0\le\eta<\infty)$ is taken to be

$$\bar{Y}=\left(\frac{(1+2\sigma)}{3}\right)\frac{1}{\xi}\left[\frac{1}{(1+\frac{1}{4}\eta^2)^{2\sigma}}\right] \tag{37}$$

This solution is recognized as a modified form of Peters' solution for a passive scalar in the circular jet flow geometry.[10] If it is taken that $Y_F(\xi,0)=Y_{Fj}$, $Y_O(\xi,0)=0$ for $0\le\xi\le1$, i.e., there is no combustion on the centerline upstream of the "effective jet exit,"[4] then, for this formulation, it is required that $C_i=1$ and/or $\sigma=1$.

If an effective flame for the turbulent flow is defined by the locus $Y_O=Y_F$, then $\bar{Y}=\bar{Y}_f=(Y_{O\infty}/(Y_{Fj}+Y_{O\infty}))$ and the "shape" of the flame, for $\sigma=1$, is given by

$$\eta_f(\xi;\xi_f)=2\left[\left(\frac{\xi_f}{\xi}\right)^{1/2}-1\right]^{1/2} \tag{38a}$$

where ξ_f, the "length" of the flame (i.e., $\xi=\xi_f$ for $\eta_f=0$), is given by

$$\xi_f=\left(\frac{(Y_{Fj}+Y_{O\infty})}{Y_{O\infty}}\right) \tag{38b}$$

Consider now the behavior of Y_F. With $\sigma_i\simeq\sigma=1$, D'', $B''=$(specified) constants, etc., the initial/boundary-value problem for Y_F is given by Eq. (15), with $i=F$, and the *pertinent* boundary/initial conditions of Eqs. (17-19). For Y_F of the form

$$Y_F(x,z)=X(\xi,\eta) \tag{39}$$

the initial/boundary-value problem for $X(\xi,\eta)$ in the domain $(0<\eta<\infty, 1<\xi<\infty)$ can be written as

$$\frac{\partial}{\partial\eta}\left(\eta\frac{\partial X}{\partial\eta}\right)+\frac{\eta^2}{(1+\frac{1}{4}\eta^2)}\frac{\partial X}{\partial\eta}-\frac{2\xi\eta}{(1+\frac{1}{4}\eta^2)^2}\frac{\partial X}{\partial\xi}$$
$$=2(\gamma''B'')\frac{\eta^2}{(1+\frac{1}{4}\eta^2)^3}$$
$$\times\left(X\left[Y_{O\infty}-\left\{\frac{(Y_{Fj}+Y_{O\infty})}{\xi(1+\frac{1}{4}\eta^2)^2}-X\right\}\right]\right) \tag{40a}$$

$$X\to0 \text{ as } \eta\to\infty, \frac{\partial X}{\partial\eta}\to0 \text{ as } \eta\to0 \tag{40b}$$

$$X\to X_i=\frac{Y_{Fj}}{(1+\frac{1}{4}\eta^2)^2}\quad \text{as } \xi\to1 \tag{40c}$$

It can be shown (see Ref. 1) that, consistent with the previously introduced approximations of this formulation, Eq. (40c) is the appropriate initial condition for this initial/boundary-value problem.

IV. Numerical Solutions

Under the transformation

$$(\xi,\eta)\to(t,\eta) \quad (41)$$

with $t=\log\xi$, the initial/boundary-value problem of Eq. (40) for the determination of $X(t,\eta;\ldots)$ in the domain $(t\geq 0,\eta\geq 0)$ can be written as

$$\frac{\partial X}{\partial t}=\frac{1}{2}\left(1+\frac{1}{4}\eta^2\right)^2\left(\frac{\partial^2 X}{\partial\eta^2}+\frac{1}{\eta}\frac{\left(1+\frac{5}{4}\eta^2\right)}{(1+\frac{1}{4}\eta^2)}\frac{\partial X}{\partial\eta}\right.$$

$$-(\gamma''B'')\frac{\eta}{(1+\frac{1}{4}\eta^2)}$$

$$\left.\times\left(X\left[Y_{O\infty}-\left\{\frac{(Y_{Fj}+Y_{O\infty})\exp(-t)}{(1+\frac{1}{4}{}^2)^2}-X\right\}\right]\right)\right) \quad (42a)$$

$$X\to\circ \text{ as } \eta\to\infty, \frac{\partial X}{\partial\eta}\to 0 \text{ as } \eta\to 0 \quad (42b)$$

$$X\to\frac{Y_{Fj}}{(1+\frac{1}{4}\eta^2)^2} \text{ as } t\to 0 \quad (42c)$$

The initial/boundary-value problem is written now in the form adopted for the numerical solution of problems involving nonlinear parabolic partial differential equations by the method of Sincovec and Madsen.[11] With the specification of the parameters Y_{Fj}, $Y_{O\infty}$, and $(\gamma''B'')$, Eq. (42) can be solved to yield $X(t,\eta;\ldots)$ and, in turn, $Y_F(t,\eta;\ldots)$, $Y_O(t,\eta;\ldots)$, where

$$Y_F=X \quad (43a)$$

$$Y_O=\left[Y_{O\infty}-\left\{\frac{(Y_{Fj}+Y_{O\infty})\exp(-t)}{(1+\frac{1}{4}\eta^2)^2}-X\right\}\right] \quad (43b)$$

Further, with the specification of the parameters T_j $(=1)$ and Q, $T(t,\eta;\ldots)$ is determined from Eq. (22), i.e.,

$$T=\left[1+Q\left\{\frac{Y_{Fj}\exp(-t)}{(1+\frac{1}{4}\eta^2)^2}-X\right\}\right] \quad (44)$$

It is the solutions for $Y_F(x,r;\ldots)$, $Y_O(x,r;\ldots)$, and $T(x,r;\ldots)$ that are desired, however. To obtain these solutions, it is necessary to determine the inverse transformations for the independent variables. It is found that for $T_j=1$ these inverse transformations are

$$x(t;\ldots)=x_i\exp(t)=[(3/16)^{1/2}\gamma'']\exp(t) \quad (45a)$$

$$r(t,\eta;\ldots)=\left[(3/8)\int_0^\eta T(t,\eta';\ldots)\eta'\mathrm{d}\eta'\right]^{1/2}\exp(t) \quad (45b)$$

Thus, the specification of the parameters γ'' and/or x_i is also required.

The case chosen for numerical study is that of a turbulent jet of carbon monoxide gas at room temperature exhausting into stagnant air. Accordingly, the following parametric values are assigned:

$$Y_{Fj}=1.56,\ Y_{O\infty}=0.638;\ T_j=1,\ Q=14.9 \quad (46a)$$

For these parametric values, the adiabatic flame temperature is

$$T_{af}=1+Q\frac{Y_{Fj}Y_{O\infty}}{(Y_{Fj}+Y_{O\infty})}=7.75 \quad (46b)$$

(see Ref. 3). Based upon an analysis of experimental work for the determination of the "flame length," presented in the Appendix, here it is taken that

$$\gamma''=38.0 \text{ and/or } x_i=16.5 \quad (47)$$

From a preliminary parametric study (with respect to $(\gamma''B'')$) of the numerical solutions in the (t,η) plane, discussed in further detail in the Appendix, the temperature at the "flame tip," $T(t_f,0;(\gamma''B''),\ldots)\equiv T_f^\circ((\gamma''B''),\ldots)$, is determined. From this determination, it is found that $T_f^\circ=5.67$ (see Ref. 5) if the following value of the reaction parameter is assigned:

$$(\gamma''B'')=12.25 \quad (48)$$

For the values of the parameters assigned in Eqs. (46-48), the numerical solutions for $Y_F(x,r)$ and $Y_O(x,r)$ are presented in Fig. 1 and those for $T(x,r)$ in Fig. 2.

The numerical determinations of the flame locus $r_f(x)$ and the maximum temperature locus $r_m(x)$ for the same values of the parameters are given in Fig. 3.

V. Results

In the previous sections, a model theoretical formulation is analyzed for the turbulent portion of the circular fuel jet exhausting into an oxidant-containing ambient, for isobaric subsonic flow under a fast direct one-step irreversible reaction between the unpremixed fuel and oxidant. In this model formulation, an explicit local algebraic (as opposed to field-type differential) expression for the mean rate of chemical reaction is adopted, i.e., this mean rate is taken to be proportional to the product of the mean mass fraction of fuel, the mean mass fraction of oxidant, and the *magnitude* of the principal mean strain rate (for the parabolic formulation appropriate to the thin shear layer considered here). Such an explicit local algebraic expression for the mean reaction rate is compatible with the adoption of an explicit algebraic (eddy viscosity) expression for the mean rate of diffusive transport.

Through the use of a modified Howarth-type coordinate transformation, involving the mean density, it is possible to correlate the compressible flow to an incompressible one. The dynamics uncouples from the energetics, and, for the fully-developed turbulent region downstream of the "break point" (or "effective jet exit" plane), as far as the velocity (Ψ and its derivatives) and passive-scalar ($\bar{Y}$) fields are concerned, the flow may be treated as if it emerged from an upstream source-singularity. In this downstream region, the velocity and passive-scalar fields satisfy (experimentally verified[7,12]) similarity concepts, in that the axial velocity U and the passive scalar $\bar{Y}$ decay (monotonically) axially, with this decay inversely proportional to the first power of the axial distance ξ; and decay (monotonically) radially, with this decay a function of the square of the similarity radial variable η. If an effective flame for the turbulent flow is defined by the locus $Y_O=Y_F$, then, from the (similarity) formulation for the passive scalar $\bar{Y}$, it is possible to obtain expressions for the "shape" of the flame $\eta_f(\xi;\xi_f)$ and the "length" of the flame ξ_f which are independent of the model adopted for the mean reaction rate. Through consideration of experimental results[7,12] for the rate of axial decay of U and $\bar{Y}$ for the nonreacting and reacting cases and those[5,12] for the "flame length," the jet growth-rate parameter γ'' for the reacting case is obtained when this parameter for the (incompressible) nonreacting case is known.[12] The rate of axial decay for the reacting case is less

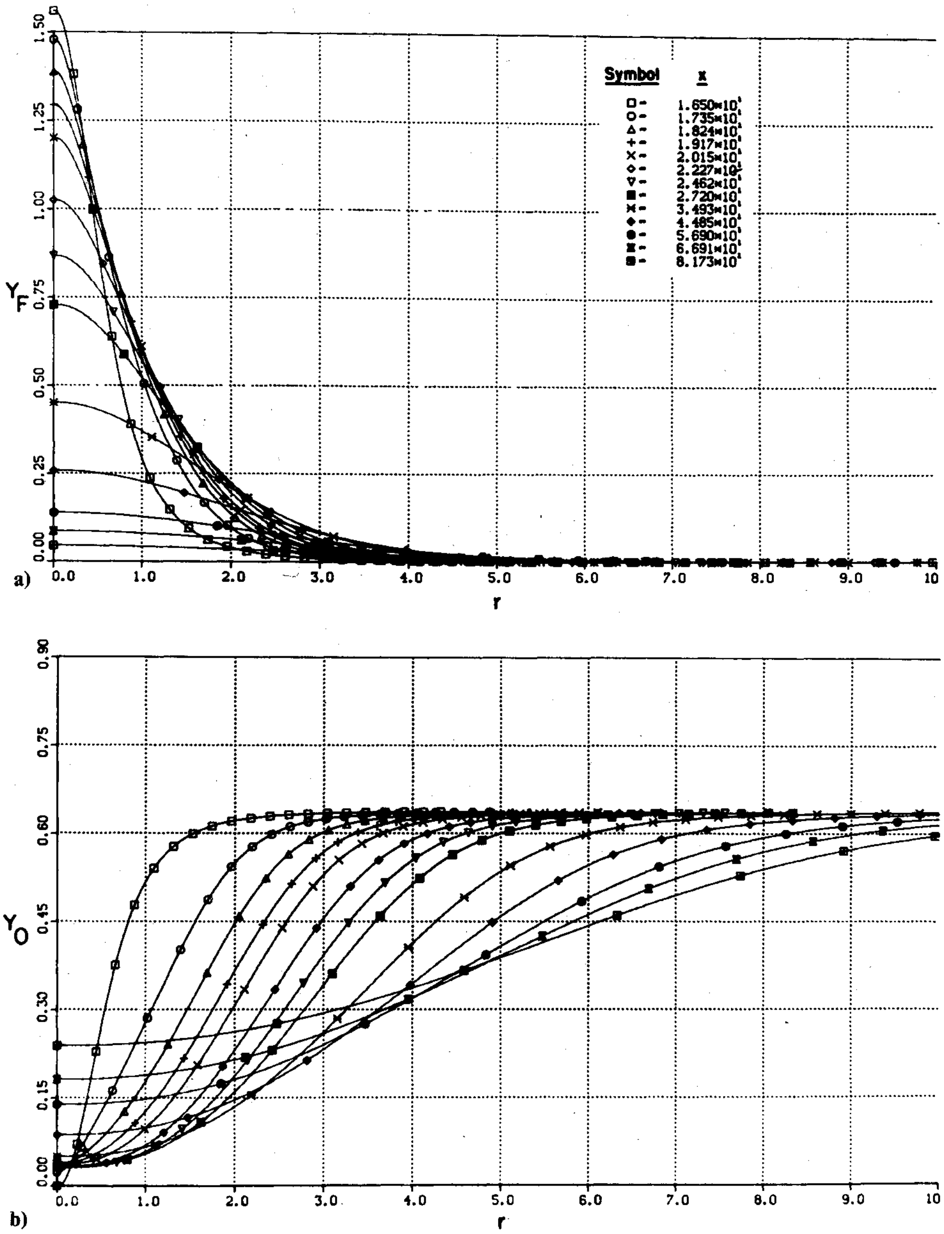

Fig. 1 Numerical solutions for circular fuel-jet species profiles: a) $Y_F(x,r)$; b) $Y_O(x,r)$. (Parameters given in Eqs. (46-48)).

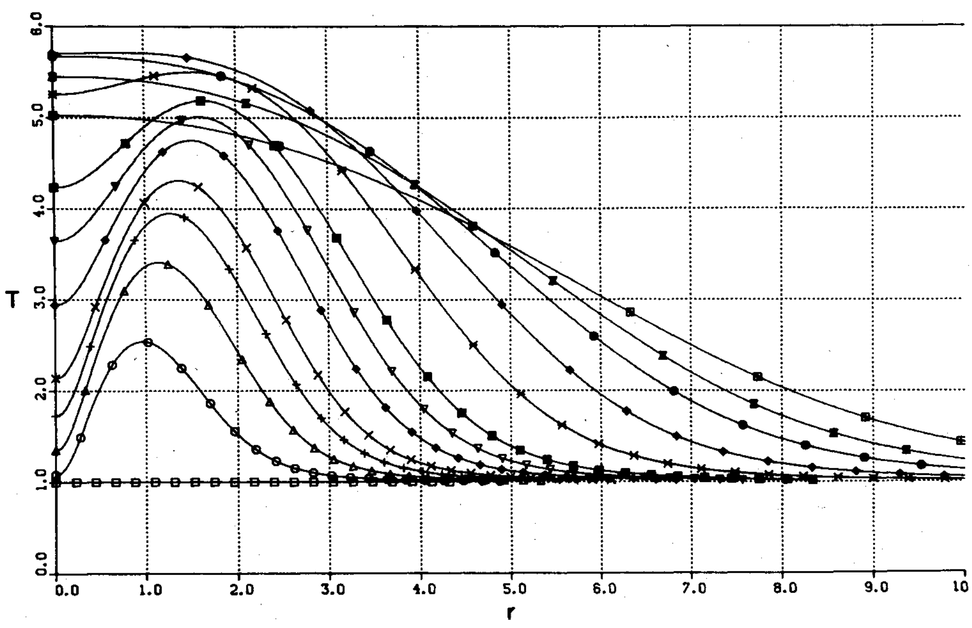

Fig. 2 Numerical solutions for circular fuel-jet temperature distribution $T(x,r)$. (Parameters given in Eqs. (46-48)).

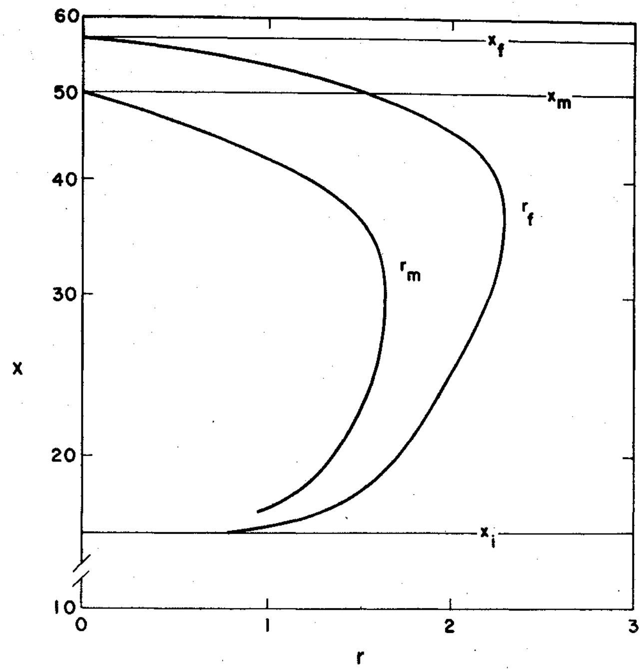

Fig. 3 Numerical solutions for the circular fuel-jet flame locus, $r_f(x)$, and maximum temperature locus, $r_m(x)$. (Parameters given in Eqs. (46-48)).

than that for the nonreacting case and, effectively, γ'' for the reacting case is greater than that for the nonreacting case.

With Ψ and its derivatives and $\bar{Y}$ determined, the (nonself-similar) initial/boundary-value problem, with the nonlinear model mean reaction-rate term as the forcing function, for the determination of Y_F, the mean mass fraction of fuel, and, in turn, $Y_{\hat{O}}$, the mean mass fraction of oxidant, and T, the temperature, is presented in the form most suitable for *numerical* solution by the method of Sincovec-Madsen.[11] This numerical method, for the solution of problems involving nonlinear parabolic partial differential equations, has been found to offer computational advantages over the (now-standard) method of Crank-Nicolson. To complete the specification of the problem, $(\gamma''B'')$, the reaction parameter, must be given. A (preliminary) parametric study of this problem yields the temperature at the "flame tip" T_f° as a function of $(\gamma''B'')$. The chosen value for $(\gamma''B'')$ is the one that produces the experimentally observed[5] value of T_f°.

The numerically determined species profiles, $Y_F(x,r)$ and $Y_O(x,r)$, are presented in Figs. 1a and 1b, respectively. From these figures, it is seen that, on the axis ($r=0$), the fuel mass fraction, $Y_F^\circ(x)$, decreases monotonically, while the oxidant mass fraction, $Y_O^\circ(x)$, increases monotonically with increasing distance downstream, x. Further, it is seen that at a fixed downstream station ($x=x^+$), the fuel mass fraction, $Y_F^+(r)$, decreases monotonically, and the oxidant mass fraction, $Y_O^+(r)$, increases monotonically with increasing radial distance from the axis, r. These numerically obtained results for $Y_F^\circ(x)$, $Y_O^\circ(x)$ and $Y_F^+(r)$, $Y_O^+(r)$ are in agreement with the experimentally observed results for these quantities.[3,5,7,13]

In a similar manner, the numerically determined results for the temperature distribution, $T(x,r)$, can be discerned from an examination of Fig. 2. The maximum temperature, $T(x,r_m(x))=T_m(x)$, is located off the axis, i.e., $r_m(x)>0$ for $x<x_m$. Both the radial position of the maximum, $r_m(x)$, and the magnitude of the maximum, $T_m(x)$, first increase (although most of the increase of $T_m(x)$ occurs at relatively small x), then decrease, with increasing axial distance downstream. The numerical results for $r_m(x)$ are presented explicitly in Fig. 3. $T_m(x)$ peaks at a value below the adiabatic flame temperature at the downstream station, $x=x_m$, at which the maximum goes to the axis, i.e., $r_m(x_m)=0$, $T_m(x_m)=T_m^\circ$, and then decreases appreciably with farther downstream distance. The temperature on the axis ($r=0$), $T^\circ(x)$, rises monotonically with increasing x, until the maximum, T_m°, is achieved at the station $x=x_m$; then decreases monotonically farther downstream. Again, these numerically obtained results for $T_m(x)$ and $T^\circ(x)$ are in agreement with the experimentally observed results for these quantities.[5,7,13]

Figure 3 presents the numerically determined flame locus, $r_f(x)$, and the maximum temperature locus, $r_m(x)$. It is seen that $r_f(x)$ first increases (from its initial off-axis location, $r_f(x_i)>0$) with downstream distance x, then decreases to the axis, i.e., $r_f(x_f)=0$. The distance downstream at which the flame contour goes to the axis, x_f, defines the "flame tip" location or "flame length." Further, the flame contour, $r_f(x)$, envelops the maximum temperature contour, $r_m(x)$, that is, the flame contour relative to the maximum temperature contour lies at a larger radial position at all downstream stations, such that $r_f(x^+)>r_m(x^+)$; and goes to the axis farther downstream, such that $x_f>x_m$. Experimental results for $r_f(x)$, x_f and $r_m(x)$, x_m have been obtained.[5,13] The numerical results for these contours are in both qualitative and quantitative agreement with these experimental results.

Thus, the capacity of this (relatively) simple theoretical model to treat the turbulent portion of the circular fuel jet is demonstrated. Development of the present model initial/boundary-value problem requires the specification of two empirical factors: γ'', the jet growth-rate parameter, and $(\gamma''B'')$, the reaction parameter; and it is shown how these parameters can be evaluated from available experimental data. The numerical solutions of this problem, whose essential feature is the explicit local algebraic expression for the mean reaction rate, are in both qualitative and quantitative agreement with the experimental results for the pertinent flow variables in this flow geometry.

The ability of this model to treat a turbulent diffusion flame for the circular-jet and the planar-jet[1] configurations, with their planes of antisymmetry for the principal mean strain rate, and to treat such a flame for the mixing-layer[2] configuration, with its plane of symmetry, suggests that the model can treat a turbulent diffusion flame in other flow configurations.

Appendix

Jet Growth-Rate Parameter

In Sec. III, it is determined that, in the domain ($1\le\xi<\infty$, $0\le\eta<\infty$), the appropriate representations for the axial component of the velocity U and the (modified) mass-fraction Shvab-Zeldovich function $\bar{Y}$ are, for $\sigma=1$,

$$U,\bar{Y}=\frac{1}{\xi}\left[\frac{1}{(1+\frac{1}{4}\eta^2)}\right] \tag{A1}$$

Thus, at the centerline ($\eta=0$),

$$U^\circ,\bar{Y}^\circ=\frac{1}{\xi}=\frac{x_i}{x}=\frac{(3/16)^{1/2}\gamma''}{x} \tag{A2}$$

for $T_j=1$. These results indicate that the ratios of the reacting and inert centerline velocities and Shvab-Zeldovich functions are

$$(U^\circ{}_{\text{react}}/U^\circ{}_{\text{inert}}),(\bar{Y}^\circ{}_{\text{react}}/\bar{Y}^\circ{}_{\text{inert}})$$

$$=((x_i)_{\text{react}}/(x_i)_{\text{inert}})=(\gamma''{}_{\text{react}}/\gamma''{}_{\text{inert}}) \tag{A3}$$

Experimentally, it has been determined[7] that

$$((x_i)_{react}/(x_i)_{inert}) \approx 5/2 \Rightarrow (\gamma''_{react}/\gamma''_{inert}) \approx 5/2 \qquad \text{(A4)}$$

For the inert case, the spreading parameter is $\gamma''_{inert} \approx 15.2$.[12] Based upon the ratio of Eq. (A4), it follows that the result for the reactive case is $\gamma''_{react} \approx 38.0$. The corresponding values for x_i are $(x_i)_{inert} \approx 6.6$; $(x_i)_{react} \approx 16.5$. This increase in γ'' (and/or x_i) for the reacting case (over that for the inert case) indicates a decrease in the axial decay of the velocity and of the passive scalar.

From Eq. (38b), the "flame length" is, for $\sigma = 1$,

$$x_f = x_i \xi_f = x_i \left(\frac{(Y_{Fj} + Y_{O\infty})}{Y_{O\infty}} \right) \qquad \text{(A5)}$$

where it is understood that $x_i = (x_i)_{react}$. For the assigned values of Y_{Fj} and $Y_{O\infty}$ given in Eq. (46), $\xi_f = 3.45$, $t_f = \log \xi_f = 1.238$, and

$$x_f = 56.9 \text{ for } x_i = 16.5 \text{ (and/or } \gamma'' = 38.0) \qquad \text{(A6)}$$

The value proposed in Ref. 5 for the "flame length" for the circular carbon monoxide jet is $x_f = 57$. This evidence indicates that for the reactive case the parametric values $\gamma'' = 38.0$ and/or $x_i = 16.5$ should be assigned.

Reaction Parameter

With the specification of Y_{Fj}, $Y_{O\infty}$, and T_j, Q (see Eq. (46)), from Eqs. (41-44), it is possible to carry out a parametric study (with respect of $(\gamma''B'')$) to determine $Y_F(t,\eta;(\gamma''B''))$, $Y_O(t,\eta;(\gamma''B''))$, and $T(t,\eta;(\gamma''B''))$. In particular, from such a study, it is possible to determine the centerline temperature, $T(t,0;(\gamma''B'')) \equiv T^\circ(t;(\gamma''B''))$; the temperature of the "flame tip," $T^\circ(t_f;(\gamma''B'')) \equiv T_f^\circ((\gamma''B''))$; and the location and magnitude of the maximum centerline temperature, $t_m = t_m((\gamma''B''))$, and $T^\circ(t_m;(\gamma''B'')) \equiv T_m^\circ((\gamma''B''))$, respectively.

In Sec. IV, detailed calculations are presented for the case of $(\gamma''B'') = 12.25$, since, for this value of $(\gamma''B'')$, the parametric study yields $T_f^\circ = 5.67$, the value proposed in Ref. 5 for the carbon monoxide fuel jet case. Further, for this value of $(\gamma''B'')$, it is determined from the study that $t_m = 1.102$, $T_m^\circ = 5.72$, and that the following ratios hold:

$$\frac{t_m}{t_f} = \frac{1.102}{1.238} = 0.890 \Rightarrow \frac{x_m}{x_f} = \frac{49.6}{56.9} = 0.872 \qquad \text{(A7a)}$$

$$\frac{T_m^\circ}{T_f^\circ} = \frac{5.72}{5.67} = 1.009 \qquad \text{(A7b)}$$

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