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THEORETICAL STUDY OF REACTIVE AND NONREACTIVE TURBULENT COAXIAL JETS

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16. Abstract

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THEORETICAL STUDY OF REACTIVE AND NONREACTIVE
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SUMMARY

The hydrodynamic properties and the reaction kinetics of axisymmetric coaxial turbulent jets having steady mean quantities are investigated in this work. From the analysis, limited to free turbulent boundary-layer mixing of such jets, it is found that the two-equation model of turbulence is adequate for most nonreactive flows. For the reactive flows, where an allowance must be made for second-order correlations of concentration fluctuations in the finite-rate chemistry for initially inhomogeneous mixture, an equation similar to the concentration fluctuation equation of Spalding's model is suggested. This equation is much simpler to use than a similar proposal by Donaldson. For diffusion limited reactions, the eddy-breakup model based on concentration fluctuations is found satisfactory and simple to use. The theoretical results obtained from these various models are compared with some of the available experimental data.

INTRODUCTION

There are many practical applications of free turbulent mixing flow phenomena. For instance, the design of combustors for advanced aircraft (where weight and length should be minimized without the loss of combustion efficiency), jet ejectors, wakes behind airplanes and submarines, cooling water and waste dispersal in rivers, chimney plumes, and jet streams in the atmosphere are a few examples where the role played by free turbulent mixing is very important. Attention in this study is restricted to free turbulent boundary-layer mixing of reactive and nonreactive coaxial jets, even though many of the "real world" examples do not fit this description. The word "free" is used for the flows remote from walls. The word "boundary layer" is applied to the flow regions where a single predominant direction of flow exists and in which shear stresses, heat fluxes, and diffusion fluxes are significant only in directions at right angles to the predominant direction.

Because of the practical importance of free turbulent boundary layers, a method for reliable prediction of these flows is greatly needed. Since Reynolds (ref. 1) formulated the equations of turbulent flow almost a century ago, various investigators have attempted to construct a model of shear flows based on a closure of these equations. The general approach, involving a modeling of appropriate terms in the equations for second-order correlations of fluctuating quantities, has been pursued in detail by Rotta (ref. 2) among others. More recently Donaldson and his colleagues (ref. 3) have attempted to develop a second-order closure model that can handle with one invariant model the classical as well as nonclassical shear layer problems (examples of the latter are generation of turbulence by the atmosphere and dispersal of chemically active species in the Earth's atmosphere). They attempted in references 4 and 5 to couple their invariant diffusion model to the chemistry model. In the course of the analysis, they point out the situations for which second-order correlations involving concentration fluctuations are important and must be accounted for. In cases where the reaction rates are fast and the scale of turbulence is large, the reaction model based on mean-value chemistry can be substantially in error. An extreme case would be the flow of material by a given point such that large scale discrete parcels of the reactants alternately pass the point. For such a case, half of the time the flow is all one reactant and the other half of the time it is all the other reactant. In this admittedly hypothetical case, little or no reaction is possible, although mean-value chemistry will predict one. For such a poorly mixed system, the rate of removal of the reactants from the flow will be only weakly influenced by reaction rates and will instead be limited by molecular diffusion. On the other hand, if the scale of turbulence is small enough and the reaction rates are slow enough, diffusion is always fast enough to keep the reactants well mixed. For this case the depletion of reactants will, of course, be governed by reaction rates. In many laboratory flows, the diffusive scale of turbulence is small; hence, the mean-value chemistry model may be employed. However, if the laboratory experiment is increased in size and the rest of the parameters held constant, the character of the flow will change because the scale of turbulence increases linearly with the size of the apparatus (ref. 6).

Therefore, it is clear that for chemically active turbulent flows one has to be very careful in treating the second-order correlations involving the concentration fluctuation $\left(\overline{c_i' c_j'}\right)$. However, in searching for a coupled turbulent diffusion and chemistry model which also allows for treatment of the concentration fluctuation or the "mixedness" term $\overline{c_i' c_j'}$, one has to look for a model which is acceptable in terms of the required accuracy as well as the effort and expense involved. The model proposed by Donaldson and his colleagues does not yet meet these requirements. Moreover, as they have also pointed out, the results obtained with their model should be used with caution because the length scale Λ employed in the calculation has a constant value. Their published results

so far are only pertinent where the equilibrium turbulence field is coupled to the chemistry model. In view of these limitations and because of the complexity of their closure technique, an alternate approach with reasonable simplicity of computation and, as will be shown, adequate physics of the problem has been developed in this paper.

In his study on turbulent flows with chemical reactions, Borghi (ref. 7) clearly points out the need for the modification of the molecular reaction rates by the concentration fluctuations. However, his approach also has the limitation similar to that of references 3 to 5, namely, the complexity of closure technique for second-order moments. Also, a simple mixing-length hypothesis for the turbulence model has been employed in the analysis.

Since the model presented herein is based on Spalding's work (ref. 8), his contribution will be described in detail. The Spalding three-equation $\left(E_k Wg\right)$ model, which solves the transport equations for turbulent kinetic energy E_k, variance of the fluctuations of the vorticity W of the fluid (which may also be regarded as the length scale equation), and the variance of the fluctuating component of the mass fraction of the injected reactant g, appears to meet the requirements outlined earlier with adequate representation of the turbulent flow field. These equations are solved simultaneously with those governing the mean flow behavior. At a conference devoted to comparison of the predictions of various models (for nonreactive free turbulent shear flows) with each other and with experiment, Launder, Morse, Rodi, and Spalding (ref. 9) presented the results of the energy-dissipation $\left(E_k\epsilon\right)$ model. Here ϵ represents dissipation rate of the turbulence kinetic energy. They conclude that the $E_k\epsilon$ model is surpassed only by more complex "Reynolds stress" models, which are still not completely developed. In the $E_k\epsilon$ model the two transport equations to be solved are for E_k and $\epsilon = E_k^{3/2}/l$, whereas in the $E_k W$ model the two turbulence quantities employed are E_k and $W = E_k/l^2$. (The symbol l indicates the length scale of turbulence.) There is little difference in the results using these two models for boundary-layer flows. For general flows, however, the $E_k\epsilon$ model is preferred (ref. 10).

For round turbulent free jets, Spalding (ref. 8) has added a third equation for concentration fluctuations to his $E_k W$ model. With this three-equation $E_k Wg$ model, Spalding has predicted concentration fluctuations that are in good agreement with experimental data for steady injection into a reservoir containing stagnant fluid of equal density.

In the present treatment, a fourth equation, analogous to Spalding's equation for the variance of fluctuating component of the mass fraction of injected fluid, is proposed and used to predict the mixedness term $\overline{c_i' c_j'}$. It is thought that the present four-equation model $\left(\text{i.e., the Spalding three-equation model plus the equation for the mixedness term } \overline{c_i' c_j'}\right)$ may have the potential to handle adequately reacting turbulent flows for most

cases of interest. Also, the equations involved are simpler and fewer as compared with the other existing techniques which take into account the mixedness term $\overline{c_i' c_j'}$ (the approach of ref. 4, for example). Some predictions made by using the present model are given and compared with experimental data.

For comparison with the proposed four-equation model, some results are also given by employing Prandtl's hypothesis (ref. 11) for free turbulent flows with mean-value chemistry. For fast chemical reactions and situations where the mixture is mainly composed of fragments of reactants and products, Mason and Spalding (ref. 12) have also suggested a turbulence controlled reaction model known as the eddy-breakup (EBU) model where the eddy breakup overrides chemical influence. The results from this model are included for nonpremixed reactants.

With the inclusion of the length scale equation, the four-equation model is capable of handling reacting flows with nonequilibrium turbulence. The invariant coupled diffusion and chemistry model (ref. 4) is applicable only to equilibrium turbulence fields.

The principal objectives of this investigation are briefly summarized as follows:

(1) A four-equation model for free turbulence boundary-layer mixing of reactive coaxial jets is developed and tested. Since the second-order correlations involving concentration fluctuations are important and must be accounted for in the calculation of certain reactive flows, an equation for $\overline{c_i' c_j'}$ has been included in the model along with the transport equations for E_k, W, and $\overline{c'^2}$.

(2) The existing eddy-breakup reaction model employed with the $E_k W$ turbulence model is used to test the present four-equation model in the fast reaction limit.

(3) Three versions of Prandtl's hypothesis for free turbulent flows are employed with mean-value chemistry for comparison with the models given in (1) and (2).

The present analysis has been limited to one-way forward reaction to keep the model and the calculation procedure simple. For this purpose the following reaction with mild heat release is considered:

$$NO_2Cl + NO \longrightarrow NOCl + NO_2$$

Since this reaction goes to at least 99 percent completion at about room temperature, the fluctuations in temperature or the reaction rate coefficient are not considered to be significant. The extension of the present work for a more complex reaction system with large heat release is likely to require considerable effort. Nevertheless, efforts similar to the present work should prove more practical and appealing, especially if adequate physics of turbulence is to be accounted for.

SYMBOLS

a	jet nozzle radius, meters
C	constant used in various equations
c	mass fraction of species
c_p	specific heat
D_{12}	binary coefficient of diffusion
d	jet nozzle diameter, meters
E_k	turbulent kinetic energy
g	mean-square concentration fluctuation
H	stagnation enthalpy
h	$= \sum_i c_i h_i$
h_i	enthalpy of ith species
J	turbulent flux tensor
K	thermal conductivity of mixture
k	mean reaction rate coefficient
k'	fluctuating component of reaction rate coefficient
l	local average length scale of turbulence, see equation (12)
M	molecular weight of species
M_{mix}	molecular weight of mixture
$\dot{m}_e''$	rate of mass transfer across outer boundary

N_{Le} molecular Lewis number, $\dfrac{\rho c_p D_{12}}{K}$

$N_{Le,t}$ turbulent Lewis number, $\left(\overline{v'c_i'}\Big/\overline{v'h_i'}\right)\left(\dfrac{\partial h}{\partial y}\Big/\dfrac{\partial c_i}{\partial y}\right)$

N_{Pr} molecular Prandtl number, $\dfrac{c_p \mu}{K}$

$N_{Pr,t}$ turbulent Prandtl number, $\left(\overline{v'u'}\Big/\overline{v'h_i'}\right)\left(\dfrac{\partial h}{\partial y}\Big/\dfrac{\partial u}{\partial y}\right)$

N_{Re} Reynolds number

N_{Sc} molecular Schmidt number, $\dfrac{N_{Pr}}{N_{Le}}$

$N_{Sc,t}$ turbulent Schmidt number, $\dfrac{N_{Pr,t}}{N_{Le,t}}$

p pressure

R universal gas constant

R_i rate of production of ith species

r radial coordinate

r_{ci} concentration half-radius where $c_i = \dfrac{c_{i,\mathcal{C}} + c_{i,e}}{2}$

r_u velocity half-radius where $u = \dfrac{U_{\mathcal{C}} + U_e}{2}$

S generation-dissipation term

S_D downstream component of generation-dissipation term

S_U upstream component of generation-dissipation term

T temperature

t time

U mean velocity

u	mean axial velocity
u'	fluctuating component of axial velocity
v	mean radial velocity
v'	fluctuating component of radial velocity
W	turbulent vorticity fluctuation
w'	fluctuating component of tangential velocity
x	axial coordinate
y	vertical coordinate
α	constant for external control of eddy viscosity, equations (31) to (36)
δx	forward step size in numerical solution
κ	eddy viscosity coefficient, equations (32) and (34)
$\bar{\kappa}$	eddy viscosity coefficient for Donaldson-Gray model, equations (35) and (36)
Λ	length scale, equations (23) to (29)
λ	microscale length, equations (27) to (29)
μ	laminar viscosity
μ_t	turbulent viscosity, $-\overline{u'v'}\big/\frac{\partial u}{\partial y}$
ν	kinematic viscosity
ρ	density
σ	parameter in finite-difference equation
τ	shear stress

ϕ general dependent variable

χ mole fraction

ψ stream function

ω dimensionless stream function

Subscripts:

A   species A

B   species B

chem   chemistry

$\mathcal{C}$ center line

Ek   relating to turbulent kinetic energy

e   external stream

ebu   relating to eddy-breakup model

eff   effective

i   species i

j   species j

max   maximum

o   nozzle exit plane

t   turbulent flow quantity

W   relating to turbulent vorticity fluctuation

ϕ relating to general dependent variable ϕ

8

Superscripts:

-               time mean

'   fluctuating

Chemical symbols:

NO   nitric oxide

NOCl   nitrosyl chloride

NO_2 nitrogen dioxide

NO_2Cl nitryl chloride

ANALYSIS

Time-Averaged Boundary-Layer Equations for Reactive
Axisymmetric Turbulent Flow

The following conservation equations (refs. 13, 14, and 15) govern free shear layer turbulent mixing of coflowing axisymmetric streams (fig. 1) undergoing chemical reactions:

Momentum:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = -\frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left[(\mu + \mu_t) r \frac{\partial u}{\partial r} \right] \tag{1}$$

Species:

$$\rho u \frac{\partial c_i}{\partial x} + \rho v \frac{\partial c_i}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left[\left(\frac{\mu}{N_{Sc}} + \frac{\mu_t}{N_{Sc,t}} \right) r \frac{\partial c_i}{\partial r} \right] + R_i \tag{2}$$

Energy:

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left[\left(\frac{\mu}{N_{Pr}} + \frac{\mu_t}{N_{Pr,t}} \right) r \frac{\partial H}{\partial r} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left\{ \left[\mu \left(1 - \frac{1}{N_{Pr}} \right) + \mu_t \left(1 - \frac{1}{N_{Pr,t}} \right) \right] r \frac{\partial}{\partial r} \frac{u^2}{2} \right\}$$

$$+ \frac{1}{r} \frac{\partial}{\partial r} \left[\left(\mu \frac{N_{Le} - 1}{N_{Pr}} + \mu_t \frac{N_{Le,t} - 1}{N_{Pr,t}} \right) r \sum_i h_i \frac{\partial c_i}{\partial r} \right] \tag{3}$$

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Mass:

$$\frac{\partial(\rho u)}{\partial x} + \frac{1}{r}\frac{\partial(\rho vr)}{\partial r} = 0 \tag{4}$$

In addition, for ideal reactive gases the following equation of state is also used:

$$p = \rho\left(\frac{R}{M_{mix}}\right)T \tag{5}$$

where R is the universal gas constant and M_{mix} is the molecular weight of mixture. The density fluctuations of individual species have been neglected.

The production term R_i in equation (2) may be expressed in terms of time-average and fluctuating quantities:

$$R_i = \rho\left(\frac{\partial c_i}{\partial t}\right)_{chem} = -\rho k_i\left(c_i c_j + \overline{c_i' c_j'}\right) \tag{6}$$

where it is assumed that $k_i' = 0$. This assumption is true for an isothermal system.

The following initial and boundary conditions are used to solve the conservation equations (1) to (4):

$$\left.\begin{array}{lll}
x = 0: & u = u(r) \quad c_i = c_i(r) \quad H = H(r) & \\[2ex]
r = 0: & \dfrac{\partial u}{\partial r} = \dfrac{\partial H}{\partial r} = \dfrac{\partial c_i}{\partial r} = 0 & \\[2ex]
r \to \infty: & u \to u_e \quad H \to H_e \quad c_i \to c_{i,e} &
\end{array}\right\} \tag{7}$$

For axisymmetric jets, the value of the turbulent Prandtl and Schmidt numbers is approximately 0.7 (ref. 15); this implies that the turbulent Lewis number may be taken as unity. By assuming the laminar Lewis number to be unity also, the last term in the energy equation (3) disappears. Also at low subsonic speeds, the second term on the right-hand side of equation (3) containing velocity is negligible. Thus, energy equation (3) may be simplified to

$$\rho u\frac{\partial H}{\partial x} + \rho v\frac{\partial H}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left[\left(\frac{\mu}{N_{Pr}} + \frac{\mu_t}{N_{Pr,t}}\right)r\frac{\partial H}{\partial r}\right] \tag{8}$$

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Further, in order to keep the chemistry simple, an irreversible one-step reaction of the type

$$A + B \xrightarrow{k} C + D \tag{9}$$

has been used in the computations.

For obtaining the laminar viscosity μ of gas mixtures, the following semi-empirical formula of Wilke (ref. 16) is used:

$$\mu = \sum_i \frac{x_i \mu_i}{\sum_j x_j \phi_{ij}} \tag{10}$$

where

$$\phi_{ij} = \frac{1}{\sqrt{8}}\left(1 + \frac{M_i}{M_j}\right)^{-1/2}\left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2}\left(\frac{M_j}{M_i}\right)^{1/4}\right]^2 \tag{11}$$

To complete the description of the problem, the eddy viscosity and concentration fluctuations must be specified. In the following sections several models are discussed.

Two-Equation $\left(E_k W\right)$ Model of Turbulence

The turbulence model described was developed by Spalding and his colleagues (refs. 8, 9, 10, 17, 18, and 19). It employs two parabolic partial differential equations as follows:

(1) One equation governing the distribution through the turbulent field of the specific kinetic energy of the fluctuating motion

(2) A second equation governing the distribution of a property W having the dimension of frequency squared

The quantity $W = \dfrac{E_k}{l^2}$ may be interpreted as the time-mean square (or variance) of the vorticity fluctuations. In fact, the equation employed can be for l (local average length scale of the turbulence), $E_k l$, or $E_k^{3/2}/l$ in place of the equation for $\dfrac{E_k}{l^2} = W$.

The turbulent effective viscosity is related to E_k and l by

$$\mu_t = \rho E_k^{1/2} l \tag{12}$$

with

$$E_k = \frac{1}{2}\overline{\left(u'^2 + v'^2 + w'^2\right)} \tag{13}$$

$$\ell = \left(\frac{E_k}{W}\right)^{1/2} \tag{14}$$

The equations governing E_k and W for low subsonic flows are, respectively,

$$\rho u \frac{\partial E_k}{\partial x} + \rho v \frac{\partial E_k}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_t}{N_{Pr,Ek}}\frac{\partial E_k}{\partial r}\right) + \rho E_k^{1/2}\ell\left(\frac{\partial u}{\partial r}\right)^2 - C_D\rho\frac{E_k^{3/2}}{\ell} \tag{15}$$

Advection   Diffusion   Generation   Dissipation

$$\rho u \frac{\partial W}{\partial x} + \rho v \frac{\partial W}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_t}{N_{Sc,W}}\frac{\partial W}{\partial r}\right) + \overline{C}_1\rho E_k^{1/2}\ell\left(\frac{\partial^2 u}{\partial r^2}\right)^2 + \overline{C}_3\rho\frac{E_k^{1/2}}{\ell}\left(\frac{\partial u}{\partial r}\right)^2 - \overline{C}_2\rho\frac{E_k^{1/2}}{\ell}W$$

Advection   Diffusion   Generation   Decay

$$\tag{16}$$

In these equations $N_{Pr,Ek}$ and $N_{Sc,W}$ are Prandtl and Schmidt numbers, respectively. Further, equations (15) and (16) are solved subject to the following initial and boundary conditions:

$$\left. \begin{array}{lll} x = 0: & E_k = E_k(r) & W = W(r) \\[2ex] r = 0: & \dfrac{\partial E_k}{\partial r} = \dfrac{\partial W}{\partial r} = 0 & \\[2ex] r \to \infty: & E_k \to E_{k,e} & W \to W_e \end{array} \right\} \tag{17}$$

The values of the various constants appearing in equations (15) and (16) are taken from reference 16 and are given as follows:

$$C_D = 0.09$$

$$\overline{C}_1 = 3.50$$

$$\overline{C}_2 = 0.17$$

$$\overline{C}_3 = 1.48$$

$$N_{Pr,Ek} = 0.90$$

$$N_{Sc,W} = 0.90$$

$$(18)$$

Equation (16) has been derived (ref. 20) by analogy to equation (15). The turbulent energy generation term is $\mu_t\left(\frac{\partial u}{\partial r}\right)^2$; the shear stress, $\tau = \mu_t\left(\frac{\partial u}{\partial r}\right)$. The eddy viscosity is taken equal to $\rho E_k^{1/2}l$. The dissipation is assumed proportional to $E_k^{3/2}/l$. The constant C_D is assigned a value of 0.09 to satisfy the energy equilibrium characteristics of constant stress wall layers.

Though the equations employed in the turbulence model are for E_k and W (same as E_k/l^2), other models solve for different combinations of E_k and l. For example, equations for $\epsilon = E_k^{3/2}/l$ or $E_k l$ have been employed in place of the equation for W (refs. 9 and 10). Whereas there is little difference in the results between these two models for boundary-layer flows, recent results (ref. 3) indicate that for general flows the ϵ equation is preferable to the W and $E_k l$ equations.

Correlations of Concentration Fluctuations

A third equation in the turbulence model developed by Spalding (ref. 8) to predict concentration fluctuations is given as

$$\rho u \frac{\partial g_{AA}}{\partial x} + \rho v \frac{\partial g_{AA}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\mu_t}{N_{Sc,g}} \frac{\partial g_{AA}}{\partial r}\right)$$
$$+ C_{g1}\rho E_k^{1/2}l\left(\frac{\partial c_A}{\partial r}\right)^2 - C_{g2}\rho \frac{E_k^{1/2}}{l} g_{AA} \qquad (19)$$

where

$$g_{AA} = \overline{c_A'^2} = \overline{c_A' c_A'}$$

Here $N_{Sc,g}$ has the significance of "effective Schmidt number" and has been assigned a value of 0.7 (ref. 8). The constants C_{g1} and C_{g2} are given values of 2.7 and 0.134, respectively, from reference 8.

A fourth equation similar to equation (19) is proposed for $g_{AB}\left(\overline{c'_A c'_B}\right)$:

$$\rho u \frac{\partial g_{AB}}{\partial x} + \rho v \frac{\partial g_{AB}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\mu_t}{N_{Sc,g}}\frac{\partial g_{AB}}{\partial r}\right) + C_{g1}\rho E_k^{1/2}l\left(\frac{\partial c_A}{\partial r}\right)\left(\frac{\partial c_B}{\partial r}\right) - C_{g2}\rho \frac{E_k^{1/2}}{l}g_{AB}$$

$$\underbrace{}_{\text{Advection}} \qquad \underbrace{}_{\text{Diffusion}} \qquad \underbrace{}_{\text{Generation}} \qquad \underbrace{}_{\text{Decay}}$$

(20)

The following initial and boundary conditions have been employed to solve equations (19) and (20):

$$\left.\begin{array}{lll} x = 0: & g_{AA} = g_{AA}(r) & g_{AB} = g_{AB}(r) \\[2mm] r = 0: & \dfrac{\partial g_{AA}}{\partial r} = \dfrac{\partial g_{AB}}{\partial r} = 0 & \\[2mm] r \to \infty: & g_{AA} \to (g_{AA})_e & g_{AB} \to (g_{AB})_e \end{array}\right\}$$

(21)

The values used for C_{g1} and C_{g2} appearing in equation (20) are the same as those suggested for equation (19). These values might need some change for certain reactions, since C_{g1} and C_{g2} have been chosen in reference 8 to obtain agreement with the experimental data on fluctuations of concentration of the injected fluid. However, it may be noted that C_{g1} has a value close to that of C_1 whereas C_{g2} is closer to C_2. This is to be expected in light of the similar significances of the relevant terms in the equations.

In order to compare equations (19) and (20) with those given in reference 21 (pp. 7-1 to 7-20), these equations are further simplified for the case of equilibrium turbulence. Thus, by assuming that generation of g equals dissipation of g locally, the following equations are obtained from equations (19) and (20):

$$g_{AA} = \frac{2.7}{0.134}l^2\left(\frac{\partial c_A}{\partial r}\right)^2$$

$$\overline{c'_A c'_A} = 20.149 l^2\left(\frac{\partial c_A}{\partial r}\right)^2$$

(22a)

14

$$\overline{c_A' c_B'} = 20.149 l^2 \left(\frac{\partial c_A}{\partial r}\right)\left(\frac{\partial c_B}{\partial r}\right) \tag{22b}$$

Equations (22a) and (22b) compare directly with the following equations given by Donaldson (ref. 21) for superequilibrium theory:

$$\overline{c_A' c_A'} = CC\Lambda^2 \left(\frac{\partial c_A}{\partial r}\right)^2 \tag{23}$$

$$\overline{c_A' c_B'} = CC\Lambda^2 \left(\frac{\partial c_A}{\partial r}\right)\left(\frac{\partial c_B}{\partial r}\right) \tag{24}$$

where

$$CC = 1.706$$

Equations (22a) and (22b) are equivalent to equations (23) and (24) if the length scale l used by Spalding is related to the length scale Λ used by Donaldson by the relation

$$l = 0.291\Lambda \tag{25}$$

or, in terms of Spalding's coefficient,

$$l = C_D^{1/2}\Lambda \tag{26}$$

The chemical mixedness term $\overline{c_i' c_j'}$ appearing in equation (6) is evaluated by using equation (20) rather than its simplified form (eq. (22b)).

Equations (19) and (20) can be further compared with those obtained in reference 4 for the invariant coupled diffusion and chemistry model. The authors of reference 4 have obtained equations of the following form for g_{AB} and g_{AA} for an atmospheric shear layer with constant density:

$$u\frac{\partial g_{AB}}{\partial x} = -\overline{c_A' v'}\frac{\partial c_B}{\partial y} - \overline{c_B' v'}\frac{\partial c_A}{\partial y} + \frac{\partial}{\partial y}\left(\Lambda^*\sqrt{2E_k}\frac{\partial g_{AB}}{\partial y}\right) + \nu\frac{\partial^2 g_{AB}}{\partial y^2}$$

$$- 2\nu\frac{g_{AB}}{\lambda^2} - k_A\left(c_A g_{BB} + c_B g_{AB} + \overline{c_A' c_B'^2}\right)$$

$$- k_B\left(c_A g_{AB} + c_B g_{AA} + \overline{c_A'^2 c_B'}\right) \tag{27}$$

$$u \frac{\partial g_{AA}}{\partial x} = -\overline{2c_A' v'} \frac{\partial c_A}{\partial y} + \frac{\partial}{\partial y}\left(\Lambda^* \sqrt{2E_k} \frac{\partial g_{AA}}{\partial y}\right) + \nu \frac{\partial^2 g_{AA}}{\partial y^2}$$

$$- 2\nu \frac{g_{AA}}{\lambda^2} - 2k_A\left(c_A g_{AB} + c_B g_{AA} + \overline{c_A'^2 c_B'}\right) \qquad (28)$$

where y is the vertical distance, v' is the fluctuating component of the vertical velocity, Λ^* is the scale associated with velocity diffusion terms, and λ is the dissipative scale. The quantity Λ which appears in the superequilibrium approximation (eqs. (23) and (24)) is the isotropy scale. In general, there will also be a scale Λ^{**} associated with the pressure diffusion terms in the invariant turbulence model. In a simple model all three Λ's may be taken as equal; the following relationship may be used to relate them to λ (refs. 21 and 22):

$$\lambda = \frac{\Lambda}{\sqrt{a + bN_{Re,\Lambda}}} \qquad (29)$$

where a and b are constants and $N_{Re,\Lambda}$ is a Reynolds number based on Λ and E_k.

In the analysis presented in reference 4, the third-order correlation of equations (27) and (28) has been modeled in terms of the second-order correlations. However, the results are applicable only to the case where the chemistry model is coupled to the equilibrium field of turbulence. The length scale Λ is prescribed as an algebraic value. Also, extra equations are needed for modeling $\overline{c_A' v'}$ and $\overline{c_B' v'}$ and further assumptions are made to model some of the higher-order terms appearing in these equations. In view of these assumptions and the complexity of their turbulence model, it is felt that equations (19) and (20) may be employed with lesser computational effort. Moreover, equation (19) has been used to predict (ref. 8) concentration fluctuations with good agreement with the experimental data for the case of steady injection into a reservoir containing stagnant fluid of equal density.

Eddy-Breakup (EBU) Model for Reaction Rates

For fast chemical reactions, a simpler model which adequately accounts for the fluctuations in temperature and concentrations has been proposed by Spalding (ref. 12). The model known as the eddy-breakup model involves the calculation of g_{AA} either from its differential equation (eq. (19)) or its approximate algebraic form (eq. (22a)). In this model the reactions are essentially "diffusion limited;" that is, the reaction rate is determined by the rate at which one of the reactants is supplied by diffusion rather than

by chemical kinetics. Spalding has proposed the following eddy-breakup reaction rate expression for premixed turbulent flames of high temperature:

$$R_i = -C_{ebu}\rho g_{AA}^{1/2} \frac{E_k^{1/2}}{l} \tag{30}$$

where C_{ebu} is a universal constant for high Reynolds number flow and has an approximate value of 0.53. Equation (30) is employed to model the reaction between NO_2Cl and NO, which is a quite fast reaction with mild heat release (ref. 23). For the case analyzed here, NO_2Cl and NO are not premixed. The rate prediction depends upon the concentration fluctuations of the injected reactant (NO_2Cl). However, to satisfy the requirement that no reaction is predicted whenever one of the two reactants is zero, the smaller of the NO_2Cl or NO concentration fluctuations is employed in the EBU model. Comparison of the results is made with those for the case where the reaction rates are predicted from expressions (6) and (20). The turbulence model employed with these two chemistry models is the Spalding E_kW model of turbulence.

Turbulence Models Employing Prandtl's Hypothesis

The following eddy viscosity models based on Prandtl's hypothesis for free turbulent flows were also used to predict the axisymmetric turbulent jet velocity profiles.

(1) The Ting-Libby model (ref. 24):

Initial region:

$$\left(\text{Upstream of axial position where } \frac{U_{\mathbb{C}} - U_e}{U_o - U_e} = 0.95\right)$$

$$\mu_t = \rho\epsilon = \alpha(0.00137)\left|U_o - U_e\right|\rho\left(\frac{\rho_o}{\rho}\right)^2 \tag{31}$$

Developed region:

$$\mu_t = \rho\epsilon = \alpha\kappa\bar{r}_{1/2}\left|U_{\mathbb{C}} - U_e\right|\rho\left(\frac{\rho_o}{\rho}\right)^2\left(\frac{\eta}{r}\right)^2 \tag{32}$$

where

$$\eta^2 = 2\int_0^r \left(\frac{\rho_{\mathbb{C}}}{\rho}\right)r'dr'$$

$\bar{r}_{1/2}$ value of η where $u = \dfrac{U_{\math4} + U_e}{2}$

ϵ eddy diffusivity

κ eddy viscosity coefficient given by Schlichting (ref. 10) as 0.025

Here α may be used to change the value of κ.

(2) The Ferri model (ref. 25):

Initial region:

$$\mu_t = \rho\epsilon = \alpha(0.00137)\left|\rho_{\math4}U_{\math4} - \rho_e U_e\right| \tag{33}$$

Developed region:

$$\mu_t = \rho\epsilon = \alpha\kappa b_{1/2}\left|\rho_{\math4}U_{\math4} - \rho_e U_e\right| \tag{34}$$

In equation (34), $b_{1/2}$ is the value of r where

$$\rho u = \frac{\rho_{\math4}U_{\math4} + \rho_e U_e}{2}$$

(3) The Donaldson-Gray model (ref. 26):

Initial region:

$$\mu_t = \rho\epsilon = \alpha\bar{\kappa}\left(r_{1/2} - r_i\right)\rho\frac{\left|U_{\math4} - U_e\right|}{2} \tag{35}$$

For subsonic flows, $\bar{\kappa} = 0.0468$. In equation (35), $r_{1/2}$ is the value of r where $u = \dfrac{U_{\math4} - U_e}{2}$ and r_i is the inner mixing-zone radius defined as the value of r where

$$\frac{u - U_e}{U_o - U_e} = 0.95$$

Developed region:

$$\mu_t = \rho\epsilon = \alpha\bar{\kappa}r_{1/2}\rho\frac{\left|U_{\math4} - U_e\right|}{2} \tag{36}$$

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These three eddy viscosity models predict the potential core and the axial decay with very little difference. In this work, however, the Donaldson-Gray model is used for comparisons with the two-equation model. All these models are, of course, coupled to the chemistry models in which reaction rates are specified by simple time averaging of the instantaneous Arrhenius expression with neglect of the mixedness term $\overline{c_i' c_j'}$ and fluctuations in the reaction rate coefficient (k').

In summary, the Spalding $E_k Wg$ model (ref. 8) is investigated in detail. An extra equation analogous to Spalding's concentration fluctuation equation is added to this model to evaluate the mixedness term $\overline{c_i' c_j'}$. This along with the mean-value term is then used to evaluate the reaction rate expression from the Arrhenius rate equation. The eddy-breakup reaction model with coupling to the $E_k Wg$ model and the eddy-viscosity model based on Prandtl's hypothesis with mean-value chemistry are included for comparison only. The comparison would reflect the magnitude of error involved when Prandtl's hypothesis is employed for certain predictions.

Transformation of Equations

For the axisymmetric jet problem considered herein, it is convenient to use Von Mises transformation. The stream function can be defined from the continuity equation (eq. (4)) by its partial derivatives:

$$\left. \begin{aligned} \rho u r &= \frac{\partial \psi}{\partial r} \\[2ex] \rho v r &= -\frac{\partial \psi}{\partial x} \end{aligned} \right\} \tag{37}$$

All the differential equations of interest are parabolic partial differential equations of the form

$$\rho u \frac{\partial \phi}{\partial x} + \rho v \frac{\partial \phi}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r}\left(r J_\phi\right) + S_\phi \tag{38}$$

where

$$J_\phi = \frac{\mu_{eff}}{\sigma_\phi} \frac{\partial \phi}{\partial r}$$

By applying transformation (37) to equation (38), the following equation is obtained:

$$\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial \psi}\left(\rho u \frac{\mu_{eff}}{\sigma_\phi} r^2 \frac{\partial \phi}{\partial \psi}\right) + \frac{1}{\rho u} S_\phi \tag{39}$$

When

$$\omega = \frac{\psi}{\psi_e} = \frac{\int_0^r \rho u r \, dr}{\int_0^{r_e} \rho u r \, dr} \tag{40}$$

is introduced and

$$\frac{\partial \psi_e}{\partial x} = -r_e \dot{m}_e'' \tag{41}$$

from the definition of ψ, then equation (39) may be written as

$$\frac{\partial \phi}{\partial x} + \frac{r_e \dot{m}_e''}{\psi_e} \omega \frac{\partial \phi}{\partial \omega} = \frac{\partial}{\partial \omega}\left(\frac{r^2 \rho u}{\psi_e^2} \frac{\mu_{eff}}{\sigma_\phi} \frac{\partial \phi}{\partial \omega}\right) + \frac{1}{\rho u} S_\phi \tag{42}$$

where $\dot{m}_e''$ is the rate of mass transfer across the e boundary. (See fig. 2.) The introduction of the new variable ω, defined by expression (40), helps to keep the flow field between 0 and 1 and the number of computational points well distributed. In equation (42), the terms on the left-hand side are representative of advection by the mean flow and those on the right-hand side represent the diffusion and source/sink terms, respectively, of the entity ϕ.

Equation (42), with the reaction models given by equations (6) and (30), is solved with the help of the Patankar-Spalding GENMIX finite-difference procedure (ref. 13) with some modifications suggested in reference 27. Some of the changes are described briefly subsequently.

Predictions with the turbulent eddy-viscosity models based on Prandtl's hypothesis and the mean-value chemistry are made by employing the method of calculation of reference 28. It is a mixed implicit/explicit finite-difference scheme. In this scheme, the stability problems inherent in fully explicit finite-difference schemes are shown to be eliminated, and stable step sizes are shown to be increased by up to 4 orders of magnitude. Details of the method of calculation can be found in reference 28.

Selection of Chemicals

As pointed out in the beginning, a one-step reaction of the type $A + B \longrightarrow C + D$ has been used in the analysis to keep the chemistry simple. A reaction which falls in this category is the one between NO_2Cl and NO. The stoichiometric reaction between

NO_2Cl and NO, which goes to 99 percent completion at room temperature, is believed to proceed by way of the following one-step reaction (refs. 23, 29, and 30):

$$NO_2Cl + NO \xrightarrow{k} NO_2 + NOCl \tag{43}$$

where $k = 1.39552 \times 10^{-17}$ cm^3/molecule-sec at 300 K (ref. 23 [1]). Reference 29 points out that the forward reaction in this case is faster than the backward reaction by about 4 orders of magnitude. The progress of the reaction in equation (43) can therefore be followed by calculation or measurement of the concentration of a single species.

The four-equation theoretical model proposed in this work to allow for the mixedness term $\overline{c_i' c_j'}$, however, is not limited to irreversible bimolecular reactions. Reaction (43) has been chosen with a view to keep both the theoretical predictions as well as the experimental measurements simple. Reversible and multistep reactions may be treated by extension of the four-equation model with appropriate equations, but the validity of such modeling would first need the verification of equation (20) from measurements.

Initial Conditions

The profiles of u, E_k, and l needed to start the integration at the nozzle exit plane have not been measured in some of the experimental data included herein for comparison. Therefore, for prediction of these flows, the initial conditions were assumed as follows. The velocity profiles were taken as uniform at the exit and the streams were assumed to carry no turbulence. The calculations were started from estimated distributions of u, E_k, and l in a very thin mixing layer at the edge of the nozzle lip. In the predictions, a self-similar mixing layer evolved. Therefore, the initial distributions of u, E_k, and l in the very thin layer were found to have no appreciable influence on the downstream results. This approach was used by Rodi (ref. 31) in the prediction of nonreactive free turbulent boundary layers.

Where initial profiles of velocity at the nozzle exit plane are available, the following relation between turbulent shear stress and turbulent kinetic energy is employed (ref. 32):

$$\tau_t = 0.3 \rho E_k \tag{44}$$

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[1] The value of k given in reference 23 is incorrectly quoted in both references 29 and 30.

or from equation (12),

$$\rho E_k^{1/2} l \frac{\partial u}{\partial r} = 0.3 \rho E_k$$

or

$$E_k^{1/2} = \frac{U_o}{0.3} \frac{l}{a} \frac{\partial(u/U_o)}{\partial(r/a)} \tag{45}$$

To evaluate equation (45) at the nozzle exit plane, the length scale[2] l is taken as the constant fraction $C_1 C_7$ of the shear layer width (ref. 33) and determined by using the following formula:

$$l = C_1 C_7 |y_{0.1} - y_{0.9}| \tag{46}$$

with

$$\frac{u(y_{0.1}) - U_e}{U_{\mathcal{L}} - U_e} = 0.1$$

and

$$\frac{u(y_{0.9}) - U_e}{U_{\mathcal{L}} - U_e} = 0.9$$

In reference 33, values of 0.08 and 0.875 have been suggested for constants C_1 and C_7, respectively. Typical initial velocity profiles and the characteristic shear widths for the inner and outer regions of flow are depicted in figure 2.

Numerical Solution

The Patankar-Spalding GENMIX finite-difference procedure (ref. 13) has been employed for the solution of equation (42), with the reaction models given by equations (6) and (30). Some modifications suggested in reference 27 have been adopted to improve the accuracy of this technique. These modifications are briefly described in this section. The calculations using the turbulent eddy viscosity models based on Prandtl's hypothesis (eqs. (31) to (36)) and mean-value chemistry have been made by employing the program described in detail in reference 28.

The essence of the GENMIX program (ref. 12) is the transformation of equations (1) to (3) and equations (15), (16), (19), and (20) to the independent variables (x, ω) with ω

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[2]In this analysis, the single length scale l has been assumed to influence the magnitudes of both the transport and the dissipation processes in a fully turbulent fluid.

defined by equation (40). The details of the numerical approximation are given in reference 13, and reference 27 contains some of these details along with modifications. Some of these details are listed below:

(1) Patankar and Spalding, using a marching integration procedure, formulated a finite-difference equation by integrating equation (42) around a microcontrol volume by using a trapezoidal method of integration. This linearization between grid points in the cross-stream direction can result in large truncation errors. Especially, when there is a large rate of increase in ϕ at one grid point, then flux conservation causes a decrease in ϕ at the neighboring grid point — a physically unreasonable situation. However, a better approximation of values between grid points can be made with Taylor series expressions to form the finite-difference equations than can be made by means of linear interpolation.

(2) A variable parameter σ is included in the difference equations so that a forward difference or a central difference scheme may be adopted. The Patankar-Spalding method employs an implicit forward difference method so that $\sigma = 1$. Formally, the truncation errors are minimum for the Crank-Nicholson central difference method for which $\sigma = 0.5$. However, this may not always be true. For example, the finite-difference method for Tollmien's jet in still surroundings (ref. 34) was found to give best results (ref. 27) for large step sizes when $\sigma = 1$. This is due to the fact that, for this problem, use of the upstream value of viscosity slightly overestimates the diffusion term, whereas the calculation of $\partial^2 \phi / \partial \omega^2$ from the downstream stations results in a slight underestimation. These two effects tend to balance each other. Generally speaking, a value of σ between 0.5 and 1 may be used to minimize the calculation time for a given problem. For the axisymmetric jet analyzed herein, $\sigma = 0.5$ was employed.

(3) The decay/production term is represented in a way similar to that of the Patankar-Spalding method:

$$d = \frac{1}{\rho u} S_\phi = S_U + \sigma S_D \phi + (1 - \sigma) S_D \phi_U \qquad (47)$$

where the subscripts U and D represent upstream and downstream values, respectively.

(4) As suggested by Patankar and Spalding, a forward step size equal to a small fraction of the mixing layer thickness is used. However, when the generation-dissipation term in equation (42) becomes large compared with the diffusion and advection terms, then the following approximate equation may be used:

$$\frac{\partial \phi}{\partial x} = \frac{1}{\rho u} S_\phi \qquad (48)$$

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or, in finite-difference form, by using equation (47),

$$\phi = \frac{\phi_U\left[1 + (1 - \sigma)S_D\delta x\right] + S_U\delta x}{(1 - \sigma)S_D\delta x} \tag{49}$$

Equation (49) yields the following limit for the forward step size:

$$\delta x < \frac{1}{\sigma(S_D)_{max}} \tag{50}$$

where $(S_D)_{max}$ is the largest S_D at a given cross section. For the present problem, $(\delta x)_{max}$ has been taken as

$$(\delta x)_{max} = \frac{0.2}{\sigma(S_D)_{max}} \tag{51}$$

for the results to be accurate. For extremely fast reactions, some other measures should be taken so that the step size is not very small.

Mention must now be made of the specification of entrainment rate to avoid large inaccuracies. The advantage of the Patankar-Spalding coordinate system is that the same number of grid points may be used to cover an increasing field width as the solution proceeds downstream. This is accomplished by specifying the entrainment rate $r_e\dot{m}_e''$ in equation (42) so as to increase the mass flow under consideration with each step. The entrainment rate determines the magnitude of the advection term $\dfrac{r_e\dot{m}_e''}{\psi_e} \omega \dfrac{\partial\phi}{\partial\omega}$ in equation (42) and, therefore, influences the whole flow field. In particular, advection should be minimal in the initial development of the solution if profiles are not smooth. At the same time another condition must also be met so that the finite-difference solution correctly represents the physics of the problem; namely, at the outer free boundary of the flow, the gradient of ϕ must approach zero. These requirements on entrainment in the initial developing region of the jet can be met by providing a number of outer points with values close to the free-stream value. As the solution advances downstream, the jet spreads through these points and appreciable entrainment does not occur until significant variations appear at points adjacent to the outer boundary.

The formulas used for specification of entrainment rate are arbitrary as long as they satisfy the previously mentioned conditions. The effect of the specified entrainment rate at each step is not known until the difference equation has been solved. Therefore, the process becomes one of guesswork to meet the earlier mentioned requirements. The following procedure has been adopted herein to specify the entrainment rate: It is first

assigned an arbitrary value. If the chosen value is too small (as exhibited by the appearance of a gradient at the outer edge), it is doubled. On the other hand, if the value used for the entrainment rate is too large (as exhibited by ϕ taking negative values), it is halved.

The actual computation procedure employed in this work is outlined. After specification of the initial profiles of the dependent variables and other parameters, the dimensionless cross-stream variable ω and all functions thereof are calculated. The numerical solution is now advanced step-by-step as follows:

(a) Obtain radius r from cross-stream variable ω and density

(b) Calculate viscosity across stream from turbulence energy and length scale

(c) Calculate decay/production terms of differential equations

(d) Set forward step size and entrainment rate

(e) Calculate finite-difference coefficients

(f) Adjust boundary values and solve finite-difference equations by simple successive substitution method

RESULTS AND DISCUSSION

The predictions made by employing the various turbulence models considered are discussed for reactive and nonreactive flows and are compared with some of the available experimental data. The predictions have been made for coaxial axisymmetric jets subject to the initial conditions presented in table I.

TABLE I.- INITIAL CONDITIONS FOR TEST CALCULATIONS

Case	Inner jet	Outer jet	U_e/U_o	U_o, m/sec	Nozzle diam., cm	T_e/T_o	T_e, K	Inner jet density, kg/m^3	Outer jet density, kg/m^3
1	Krypton	Air	0.25	36.580	0.635	1	300	3.4300	1.18
2	Air	Air	.25	36.580	.635	1	300	1.1800	1.18
3	Hydrogen	Air	.33	731.707	1.270	---	---	.0818	1.18
4	NO$_2$Cl	NO	.25	36.580	.635	1	300	3.3300	1.23

Since krypton is an inert gas, the krypton-air mixing case (case 1) has been chosen to study the turbulent mixing in the absence of chemical reactions. Further, the

molecular weight of krypton approximately equals that of NO_2Cl and the molecular weight of air approximately equals that of NO. Therefore, a comparison between the nonreactive krypton-air mixing and the reactive NO_2Cl-NO mixing can tell us how the reactions can modify the mixing.

Figures 3 and 4 show results for krypton-air mixing. These figures give the center-line velocity and composition decay for the turbulence models based on Prandtl's hypothesis and the Spalding two-equation model. The three turbulence models — namely, Ferri, Ting-Libby, and Donaldson-Gray — based on Prandtl's hypothesis predict the potential core and the axial decay with very little difference. Out of these three models, the Donaldson-Gray model is used for further comparisons. The Spalding two-equation model also predicts the potential core with almost no difference. However, this model predicts faster decay in the axial values of velocity and concentration. The Spalding model is preferred in this work because further comparisons with experimental data indicate this to be a better model.

Figures 5 and 6 give the results for air-air mixing (case 2). The conditions for case 2 correspond to Forstall series E experiment (ref. 15). The initial boundary-layer profile of reference 35 is used. In figure 5(a) the experimental data of reference 15 are compared with the predictions made by using the Donaldson-Gray model. In this model a factor α is employed which may be used to change the value of the eddy viscosity coefficient κ. In addition to the usual $\alpha = 1.0$, a power-law variation of α with x/d is also incorporated. Although some improvement in the prediction of center-line velocity decay is noticeable with the use of power-law variation of α, the results with $\alpha = 1$ do not appear much different. Therefore, α will be used with a value of unity except where otherwise indicated.

In figure 5(b) the results of the calculations from different turbulence models are shown. Clearly the predictions from Spalding's two-equation model are superior to the other two models when compared with the experimental data of Forstall and Shapiro (ref. 15). The predictions from the Donaldson-Hilst invariant model have been made by Hilst. The initial turbulence for the model has been specified in the same way as that used for the two-equation Spalding model, namely,

$$\left(E_k^{1/2}\right)_{\text{initial}} = \frac{U_o}{0.3} \, (0.084) \left[\frac{\partial(u/U_o)}{\partial(r/a)}\right]_{\text{initial}}$$

The predictions with the invariant model appear unsatisfactory. It predicts almost no potential core and a very rapid decay as compared with the data of Forstall and Shapiro.

The prediction with the invariant model might be improved if some of the "constants" employed in the model are modified.

Figure 6 gives some additional comparisons for the air-air mixing case. Here the various models are used to predict the velocity half-radius r_u. Once again, the predictions from the two-equation model appear more satisfactory as compared with the invariant model or the Donaldson-Gray model.

For the hydrogen-air mixing (case 3), the two-equation model predictions are excellent. (See figs. 7 and 8.) The conditions for case 3 are the ones used in reference 36. In the initial mixing region $\left(3 \leqq \frac{x}{d} \leqq 15\right)$, when the field of turbulence is non-equilibrium, the prediction methods (such as that of the Donaldson-Gray method) without a length scale equation appear to do a poor job. This result may be because, in eddy diffusivity theories of the type of Donaldson-Gray, the turbulent transport at a point is independent of the value of transport at another point. In the two-equation model, this deficiency seems to be removed by the use of a length scale equation. For this reason the Spalding two-equation model is considered better.

The predictions for the reactive mixing of NO_2Cl-NO coaxial jets (case 4) are contained in figures 9 to 11. Figure 9 shows the axial decay of the center-line velocity and the longitudinal turbulence intensity. The Donaldson-Gray and the two-equation model of turbulence both predict the center-line velocity decay almost in the same way. Also, the inclusion or omission of the mixedness term does not influence the prediction of velocity decay. However, the mixedness term does play a significant role in the prediction of center-line composition decay as shown in figure 10. The Donaldson-Gray model, which employs the mean-value chemistry, predicts complete depletion of NO_2Cl by $\frac{x}{d} \approx 14$. The two-equation model of turbulence, with the inclusion of mixedness term in the chemistry model, predicts that NO_2Cl still has a value of about 20 percent of its nozzle concentration at $\frac{x}{d} \approx 14$. Therefore, a reaction is predicted beyond this axial location. The eddy-breakup model, which employs the expression for the eddy-breakup reaction rate to predict the diffusion limited flows with concentration fluctuations, predicts results comparable to the Spalding two-equation model employing the chemistry model with mixedness term. The mixedness terms are predicted from equation (20) which is quite simple to employ with the two-equation model of turbulence. Some accurate and careful measurements are, however, desirable to firmly establish equation (20).

The importance of retaining the mixedness term is more evident in figure 11. Without the inclusion of this term, the depletion rate of NO_2Cl is overpredicted by about 100 percent. Therefore, this term should be included in a chemistry model and comparison with experimental data is required to assess its importance.

CONCLUDING REMARKS

This investigation is concerned with the hydrodynamic properties and the reaction kinetics of axisymmetric coaxial turbulent jets. The analysis is limited to the free turbulent boundary-layer mixing of such jets.

The analysis has been carried out for the two classes of turbulence models: (1) methods based on differential-mean turbulence field without length scale equation (for example, the Donaldson-Gray model), and (2) methods based on differential-mean turbulence field with length scale equation (for example, the Spalding two-equation model). The methods of the first class are appropriate for near-equilibrium flows, whereas the methods of the second class are needed for analyzing the mixing of the nonequilibrium flows with differing scales. Predictions have been made by employing these models for a variety of reactive and nonreactive jets and comparison is made with selected experimental data. It is seen that the turbulence models (of the type of Spalding's two-equation model) with a length scale equation are adequate for most nonreactive flows of the type considered in this paper. Also, the Donaldson-Hilst invariant model needs some refinements of its "constants" to predict the axisymmetric jets analyzed here.

For the reactive flows, where an allowance should be made for the concentration fluctuations in the finite-rate chemistry for an initially inhomogeneous mixture, an equation similar to the concentration fluctuation equation of the Spalding three-equation model is suggested. This equation is much simpler to use than a similar proposal of Donaldson for an equilibrium field of turbulence.

Because of the paucity of accurate experimental data for well-defined flow fields, some experimental data with simple chemistry such as

$$NO_2Cl + NO \longrightarrow NOCl + NO_2$$

are needed to test the equation proposed in this work to study the influence of the fluctuation (or mixedness) terms.

Finally, the usefulness of the model proposed lies in handling the flows which have a chemistry classification (in relation to the molecular diffusion) in between the "fast" and "slow" regimes. These regimes have also been termed in the literature as "diffusion limited" and "reaction rate limited" regimes, respectively.

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REFERENCES

1. Reynolds, Osborne: On the Dynamic Theory of Incompressible Viscous Fluids and the Determination of the Criterion. Phil. Trans. Roy. Soc. (London), ser. A, vol. 186, 1895, pp. 123-164.

2. Rotta, J.: Statistical Theory of Inhomogeneous Turbulence — Part 1. NASA TT F-14,560, 1972. (Translated from Z. Phys., vol. 129, 1951, pp. 547-572.

3. Donaldson, Coleman duP.: A Progress Report on an Attempt to Construct an Invariant Model of Turbulent Shear Flows. Turbulent Shear Flows, AGARD-CP-93, Jan. 1972, pp. B-1 — B-24.

4. Hilst, Glenn R.; Donaldson, Coleman duP.; Teske, Milton; Contiliano, Ross; and Freiberg, Johnny: The Development and Preliminary Application of an Invariant Coupled Diffusion and Chemistry Model. NASA CR-2295, 1973.

5. Hilst, Glenn R.: Solutions of the Chemical Kinetic Equations for Initially Inhomogeneous Mixtures. AIAA Paper No. 73-101, Jan. 1973.

6. Tennekes, H.; and Lumley, J. L.: A First Course in Turbulence. MIT Press, c.1972.

7. Borghi, Roland: Computational Studies of Turbulent Flows With Chemical Reaction. ONERA T.P. No. 1383, 1974. (Presented to SQUID Working Group on Turbulent Mixing (Lafayette, Indiana), May 20-21, 1974.)

8. Spalding, D. B.: Concentration Fluctuations in a Round Turbulent Free Jet. Chem. Eng. Sci., vol. 26, no. 1, Jan. 1971, pp. 95-107.

9. Launder, B. E.; Morse, A.; Rodi, W.; and Spalding, D. B.: Prediction of Free Shear Flows — A Comparison of the Performance of Six Turbulence Models. Free Turbulent Shear Flows. Volume I — Conference Proceedings, NASA SP-321, 1973, pp. 361-426.

10. Launder, B. E.; and Spalding, D. B.: The Numerical Computation of Turbulent Flows. Comput. Methods Appl. Mech. & Eng., vol. 3, no. 2, Mar. 1974, pp. 269-289.

11. Schlichting, Hermann (J. Kestin, transl.): Boundary-Layer Theory. Sixth ed. McGraw-Hill Book Co., Inc., 1968, pp. 681-707.

12. Mason, H. B.; and Spalding, D. B.: Prediction of Reaction Rates in Turbulent Premixed Boundary-Layer Flows. Combustion Institute European Symposium 1973, F. J. Weinberg, ed., Academic Press, 1973, pp. 601-606.

13. Patankar, S. V.; and Spalding, D. B.: Heat and Mass Transfer in Boundary Layers. Second ed. Int. Textbook Co. Ltd. (London), c.1970.

14. Dorrance, W. H.:   Viscous Hypersonic Flow.   McGraw-Hill Book Co., Inc., c.1962, pp. 176-183.

15. Forstall, Walton, Jr.; and Shapiro, Ascher H.:   Momentum and Mass Transfer in Coaxial Gas Jets.   J. Appl. Mech., vol. 17, no. 4, Dec. 1950, pp. 399-408.

16. Wilke, C. R.:   A Viscosity Equation for Gas Mixtures.   J. Chem. Phys., vol. 18, no. 4, Apr. 1950, pp. 517-519.

17. Spalding, Dudley Brian: A Two-Equation Model of Turbulence.   VDI-Forsch., Heft 549, 1972, pp. 5-16.

18. Spalding, D. B.:   Mathematische Modelle turbulenter Flammen.   VDI-Berichte Nr. 146, 1970, pp. 25-30.

19. Spalding, D. B.:   Mathematical Models of Continuous Combustion Systems.   Emissions From Continuous Combustion Systems, Walter Cornelius and William B. Agnew, eds., Plenum Press, 1972, pp. 3-21.   (Presented at 15th Symposium (Warren, Mich.), Sept. 27-28, 1971.)

20. Saffman, P. G.:   A Model for Inhomogeneous Turbulent Flow.   Proc. Roy. Soc. (London), ser. A, vol. 317, no. 1530, June 1970, pp. 417-433.

21. Donaldson, Coleman duP.:   Atmospheric Turbulence and the Dispersal of Atmospheric Pollutants.   EPA-R4-73-016a, U.S. Environ. Prot. Agency, Mar. 1973.   (Available from NTIS as PB 225 524.)

22. Glushko, G. S.:   Turbulent Boundary Layer on a Flat Plate in an Incompressible Fluid.   Bull. Acad. Sci. USSR, Mech. Ser., no. 4, 1965, pp. 13-23.

23. Freiling, Edward C.; Johnston, Harold S.; and Ogg, Richard A., Jr.:   The Kinetics of the Fast Gas-Phase Reaction Between Nitryl Chloride and Nitric Oxide.   J. Chem. Phys., vol. 20, no. 2, Feb. 1952, pp. 327-329.

24. Ting, Lu; and Libby, Paul A.:   Remarks on the Eddy Viscosity in Compressible Mixing Flows.   J. Aerosp. Sci., vol. 27, no. 10, Oct. 1960, pp. 797-798.

25. Ferri, Antonio: Review of Problems in Application of Supersonic Combustion.   J. Roy. Aeronaut. Soc., vol. 68, no. 645, Sept. 1964, pp. 575-597.

26. Donaldson, Coleman duP.; and Gray, K. Evan: Theoretical and Experimental Investigation of the Compressible Free Mixing of Two Dissimilar Gases.   AIAA J., vol. 4, no. 11, Nov. 1966, pp. 2017-2025.

27. Kent, J. H.:   Turbulent Jet Diffusion Flames.   Ph. D. Thesis, Univ. of Sydney, 1972.

28. Mikatarian, R. R.; Kau, C. J.; and Pergament, H. S.: A Fast Computer Program for Nonequilibrium Rocket Plume Predictions. AFRPL-TR-72-94, U.S. Air Force, Aug. 1972. (Available from DDC as AD 751 984.)

29. Wilkins, R. A., Jr.; Dodge, M. C.; and Hisatsune, I. C.: Kinetics of Nitric Oxide Catalyzed Decomposition of Nitryl Chloride and Its Related Nitrogen Isotope Exchange Reactions. J. Phys. Chem., vol. 78, no. 21, Oct. 10, 1974, pp. 2073-2076.

30. Szabó, Z. G. (K. J. Ivin, transl.): Advances in the Kinetics of Homogeneous Gas Reactions. Methuen & Co. Ltd. (London), c.1964.

31. Rodi, Wolfgang: The Prediction of Free Turbulent Boundary Layers by Use of a Two-Equation Model of Turbulence. Ph. D. Thesis, Imperial College (London), Dec. 1972.

32. Harsha, Philip T.: Prediction of Free Turbulent Mixing Using a Turbulent Kinetic Energy Method. Free Turbulent Shear Flows. Volume I — Conference Proceedings, NASA SP-321, 1973, pp. 463-521.

33. Oh, Y. H.: Analysis of Two-Dimensional Free Turbulent Mixing. AIAA Paper No. 74-594, June 1974.

34. Abramovich, G. N.: The Theory of Turbulent Jets. M.I.T. Press, c.1963, p. 81.

35. Free Turbulent Shear Flows. Volume II — Summary of Data. NASA SP-321, 1973, pp. 36-39.

36. Chriss, D. E.: Experimental Study of the Turbulent Mixing of Subsonic Axisymmetric Gas Streams. AEDC-TR-68-133, U.S. Air Force, Aug. 1968. (Available from DDC as AD 672 975.)
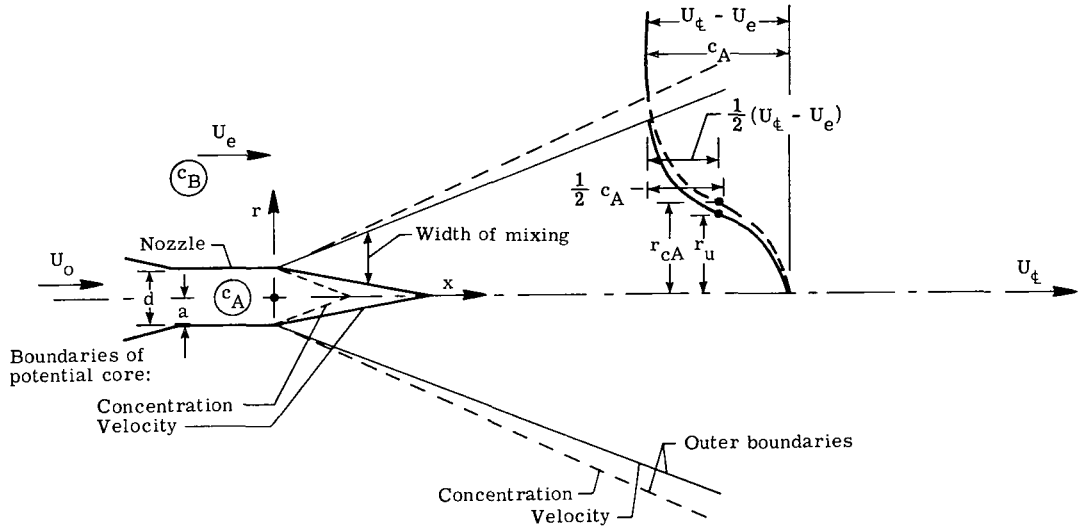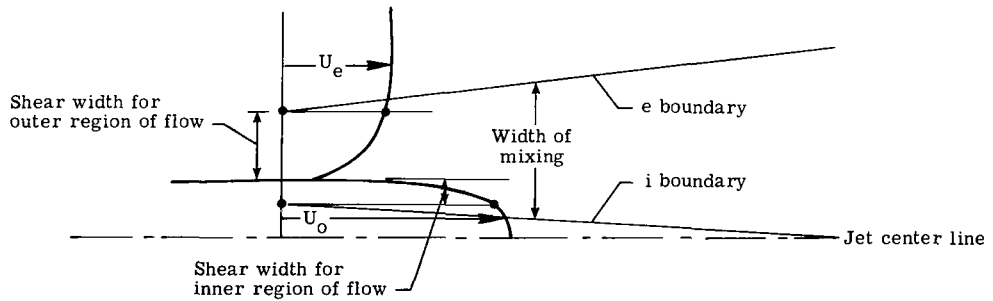
Figure 1.- Schematic of coaxial reactive jets.

Figure 2.- Initial velocity profiles and characteristic shear
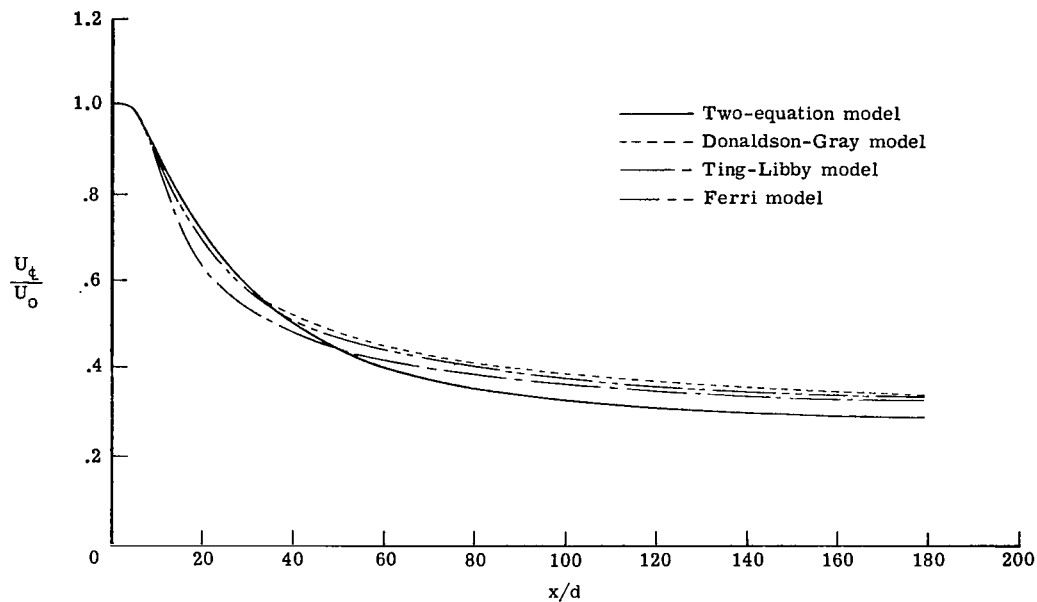widths for inner and outer regions of flow.

Figure 3.- Center-line velocity decay for krypton-air mixing
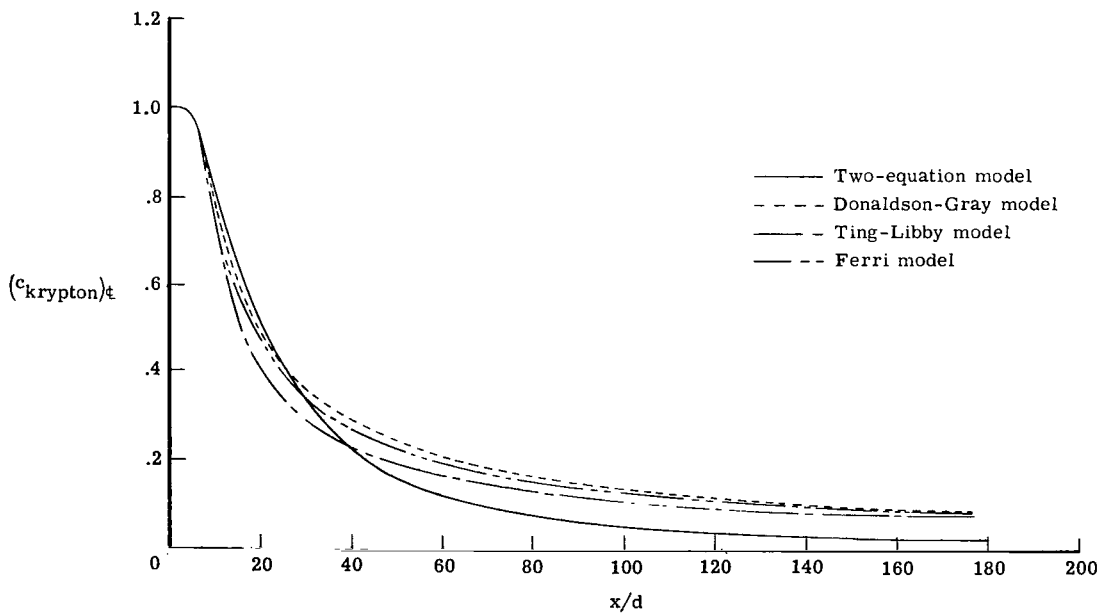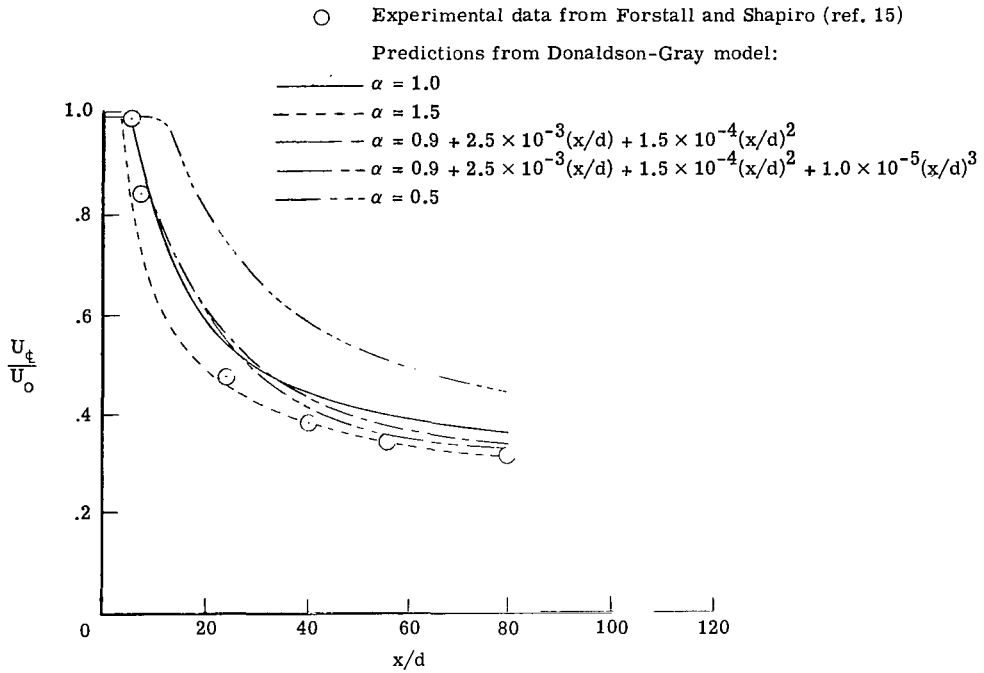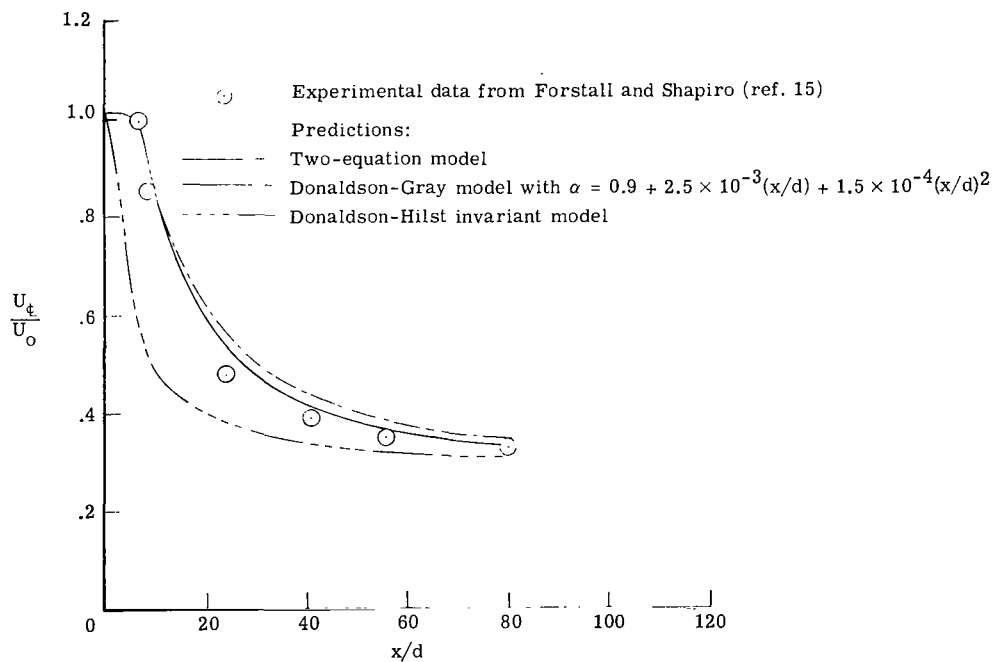with krypton injected centrally.

Figure 4.- Center-line composition decay for krypton-air mixing
with krypton injected centrally.

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(a) Comparison with predictions from Donaldson-Gray model.

Experimental data from Forstall and Shapiro (ref. 15)

Predictions:

───── Two-equation model

───── Donaldson-Gray model with $\alpha = 0.9 + 2.5 \times 10^{-3}(x/d) + 1.5 \times 10^{-4}(x/d)^2$

───── Donaldson-Hilst invariant model

(b) Comparison with two-equation, Donaldson-Gray,
and Donaldson-Hilst invariant models.
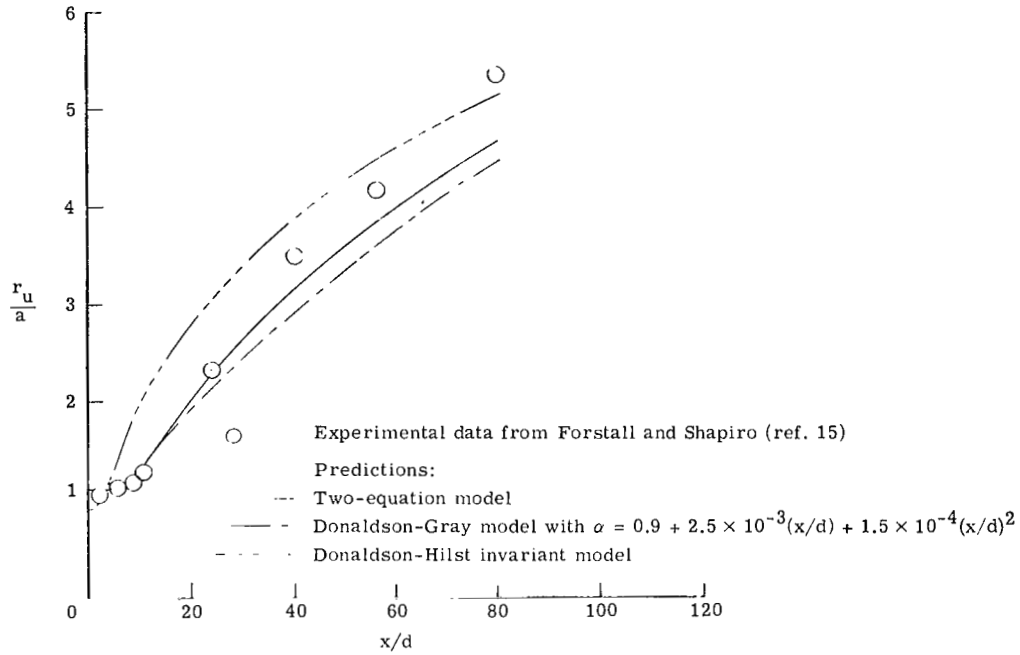
Figure 5.- Center-line velocity decay for air-air mixing.

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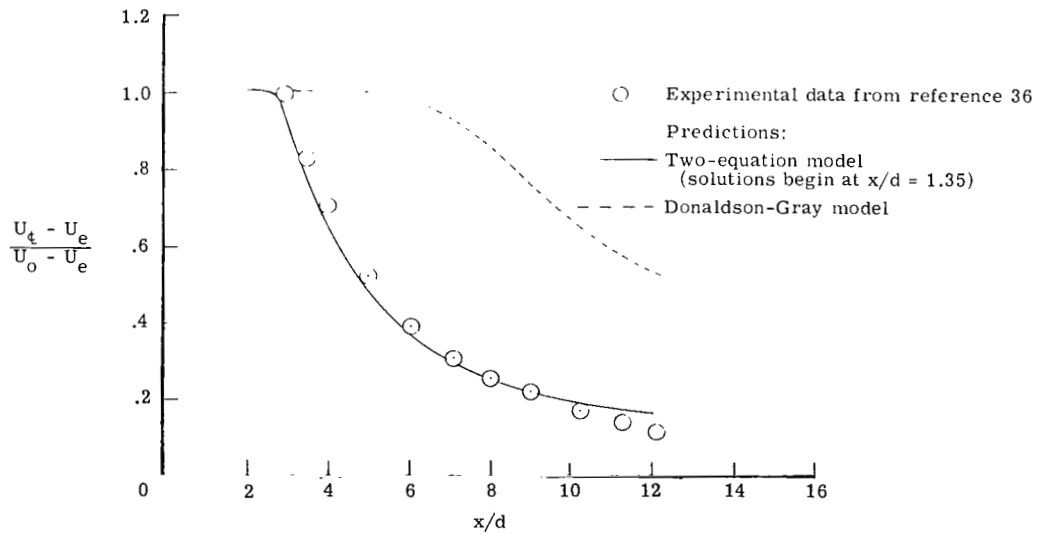Figure 6.- Axial distribution of velocity half-radius for air-air mixing.

Figure 7.- Center-line velocity decay for hydrogen-air mixing.
$U_o/U_e = 3$; $\rho_o/\rho_e = 0.08$; $\lambda = 0.24$.
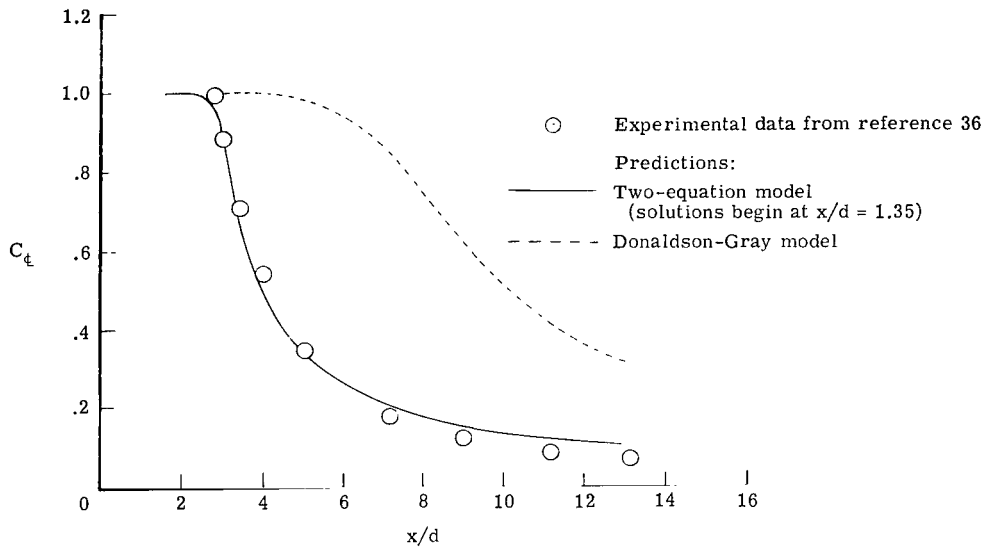
35

Figure 8.- Center-line composition decay for hydrogen-air mixing. $U_o/U_e = 3$; $\rho_o/\rho_e = 0.08$; $\lambda = 0.24$.
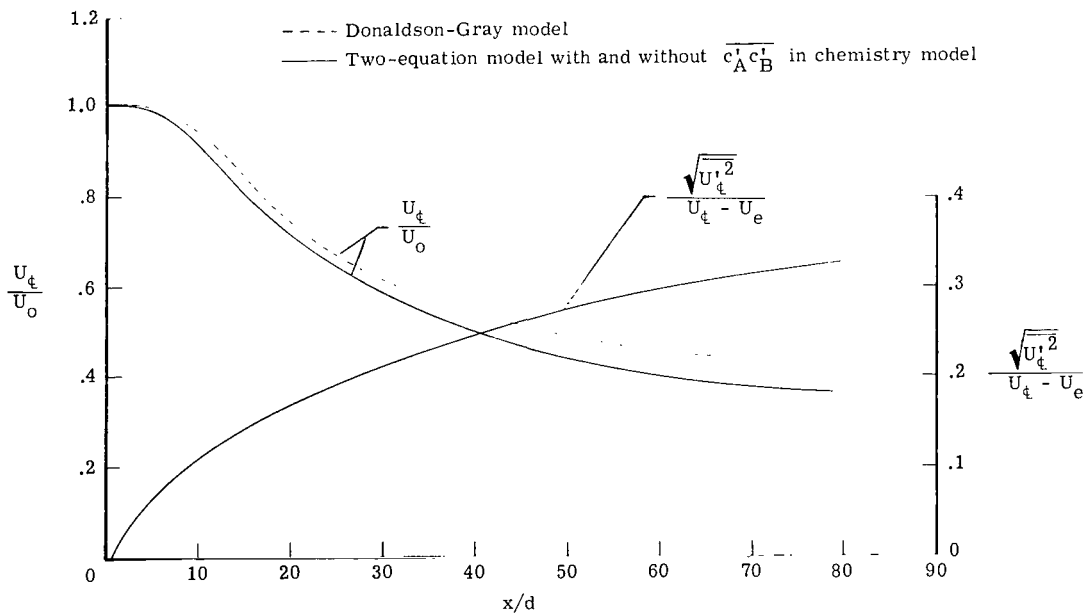

Figure 9.- Axial distribution of longitudinal turbulence intensity and center-line velocity decay for NO_2Cl-NO mixing with NO_2Cl injected centrally.
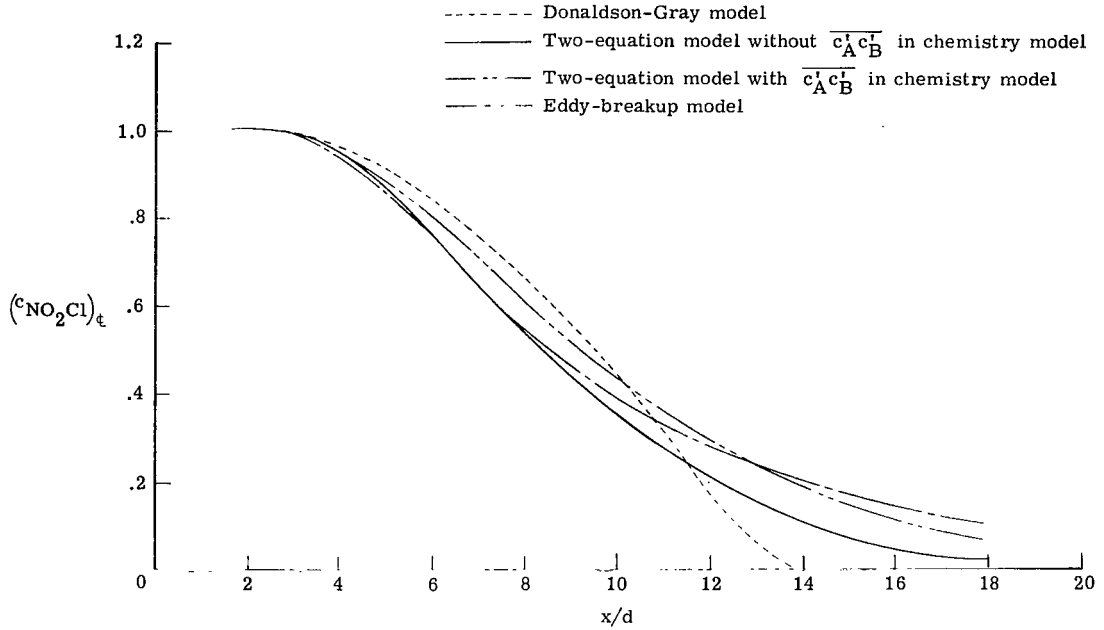
Donaldson-Gray model

Two-equation model without $\overline{c'_A c'_B}$ in chemistry model

Two-equation model with $\overline{c'_A c'_B}$ in chemistry model

Eddy-breakup model

1.2

1.0

.8

$(c_{NO_2Cl})_\ell$ .6

.4

.2

0   2   4   6   8   10   12   14   16   18   20

x/d

Figure 10.- Center-line composition decay for NO_2Cl-NO mixing with NO_2Cl injected centrally.

5

4

$\dfrac{r}{a}$ 3

2

1

x/d
○ 1
□ 10
◇ 20

With mixedness terms $(\overline{c'_A c'_B})$

Without mixedness terms $(\overline{c'_A c'_B})$

$\dfrac{\partial c_A}{\partial t} = -k_A(c_A c_B + \overline{c'_A c'_B})$

$\dfrac{\partial c_A}{\partial t} = -k_A c_A c_B$

0   100   200   300   400   500   600   700   800   900   1000   1100
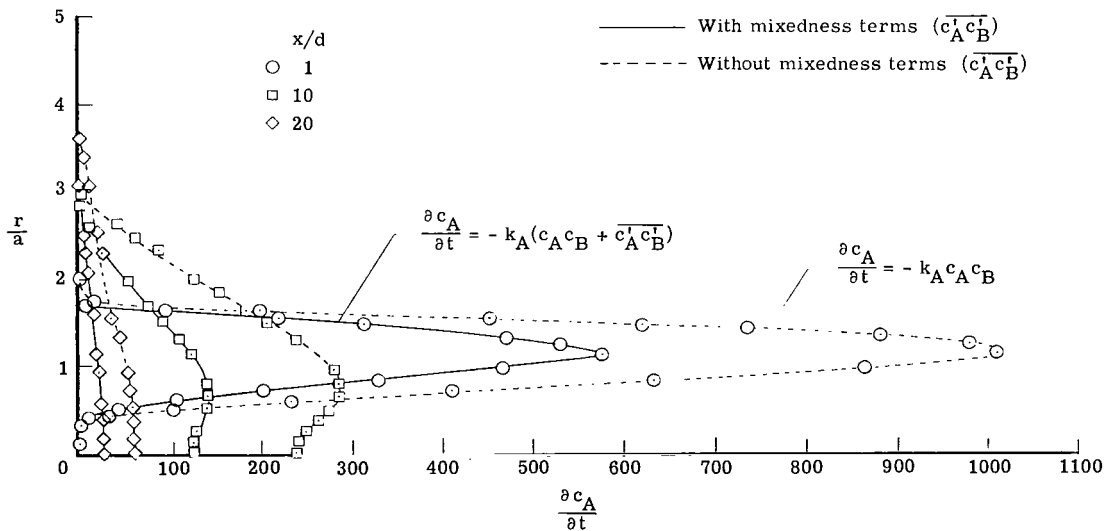
$\dfrac{\partial c_A}{\partial t}$

Figure 11.- Depletion rate of NO_2Cl at various axial locations.

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