ANALYTICAL MODELING OF FLASH-BACK PHENOMENA

BY

C. C. Feng
Trenton State College
Hillwood Lakes
P.O. Box 940
Trenton, NJ 08625

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I. Introduction

To reduce jet-engine-produced NOx and CO simultaneously, one of the advanced combustor concepts invloves lean premixed/prevaporized combustion system. In the system, since liquid fuel droplets evaporation in present-day combustion chambers is absent, locally fuel-rich and high temperature regions are removed. As a result, substantial reduction of NOx is possible without unacceptable CO emissions. Furthermore, because of lower flame temperature and more uniform combustion, smoke and radiation may be reduced, turbine inlet temperature may be improved and turbine erosion from carbon particles may be avoided.[1]

Acompanying lean premixed/prevaporized combustion system, however, are problems such as much narrower flame stabilization limit, which result in blowoff, ignition and altitude relight difficulties, and flash-back and auto-ignition, which result in the presence of flame in the premixing/prevaporizing section with potential subsequent hardware damage.[2,3,4,5,6]

To understand the flame flash-back phenomena more extensively, an analytical model has been formed and a numerical program has been written and tested to solve the set of differential equations describing the model. Initial results show that under a given set of conditions flame propagates in the boundary layer on a flat plate when the free stream is at or below 1.8 m/s. More effort is needed in working out with a turbulant reaction model and conducting various parametric studies.

The formulation of the problem, a general discussion of the finite difference solution of the governing equations and the results so far obtained and their discussion are contained in the following sections.

II. Formulation of the Problem

As shown in Figure 1, it is assumed that a uniform flow proceeds from left to right passing on top of a flat plate. Downstream a flame is established by a hot segment of the plate. Cartesian coordinates are used for the flow field.

A. Equations of Continuity and Momentum

Continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0$$

Momentum

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{1}{\rho}\left[\frac{\partial}{\partial y}\left(\mu_{eff}\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial u}{\partial x}\right)\right]$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{1}{\rho}\left[\frac{\partial}{\partial y}\left(\mu_{eff}\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial v}{\partial x}\right)\right]$$

In the above, u and v are x- and y-direction component velocities respectively, μ_{eff} is the effective viscosity which is discussed in II. E. below, ρ the density, t the time, and p the pressure.

To obtain the variation of ρ, the equation of the state is used.

B. Species Equations

$$\frac{\partial Y_i}{\partial t} + u\frac{\partial Y_i}{\partial x} + v\frac{\partial Y_i}{\partial y} = \frac{\hat{\omega}_i}{\rho} + \frac{1}{\rho}\left\{\frac{\partial}{\partial x}\left[(\rho D)_{eff}\frac{\partial Y_i}{\partial x}\right] + \frac{\partial}{\partial y}\left[(\rho D)_{eff}\frac{\partial Y_i}{\partial y}\right]\right\}$$

Where i=F (fuel) or O (oxygen); Yi is the species mass function; ρ the density, $(\rho D)_{eff}$ is the effective transport coefficient; D is the diffusion coefficient, and $\hat{W}i$ is the time-mean volumetric rate of fuel consumption depending on the combustion model described in section II. F. below.

C. Enthalpy Equation

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u h)}{\partial x} + \frac{\partial(\rho v h)}{\partial y} = \frac{\partial}{\partial x}\left[\left(\frac{\lambda}{c_p}\right)_{eff}\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[\left(\frac{\lambda}{c_p}\right)_{eff}\frac{\partial h}{\partial y}\right]$$

Where H_{fu} is the heat of combustion; c_p specific heat of the gas mixture; T the temperature and λ the conductivity; and

$h = c_p T + H_{fu} Y_F$

D. Boundary Conditions

Boundary conditions are applied at all form boundaries as described below.

Far upstream, u is specified, v is zero, the fuel fraction is 0.059, and the enthalpy is calculated from the specified heat of combustion and ambient temperature. The incoming air is stoichiometrically mixed with methane.

At the upper boundary, u, p and h have Neumann conditions, v is zero and Y_F has Dirichlet condition there.

At the lower boundary u has Neumann and Dirichlet conditions before and after the leading edge of the flat plate respectively. v is zero and p, h and Y_F have Neumann conditions except that along the hot segment of the plate h has Dirichlet condition there.

At the downstream end, v is zero, p, h and Y_F have Neumann conditions, and u is modified such that the mass flow rate is consistant with its incoming rate far upstream.

E. Transport Coefficients

It is assumed that the transport of momentum, mass and heat by molecular and turbulent mixing obeys laws of the "coefficient-times-gradient" type associated with the names of Newton, Ficks and Fourier. The subscripts "eff" implies that the turbulent fluid is being treated as a laminar one with a set of transport coefficients having augmented values. Strictly speaking, the "effective" transport coefficients may be expected to posses directional properties: for turbulence is rarely isotropic in practically interesting situations. However physical knowledge of these matters is still at an early stage. We shall assume isotropicity as frequently treated.

a) The quantity effective viscosity is defined as

$$\mu_{eff} = \mu + \mu_t = \rho(\nu + \varepsilon_H)$$

where the eddy viscosity for momentum, ε_H, assumes the well-known Prandtl mixing-length model, i.e.

$$\varepsilon_H = \ell^2 \left|\frac{\partial u}{\partial y}\right|$$

where ℓ is the mixing length and, in the viscous region, it is expressed, according to Van Driest[7], by

$$\ell = k y \left[1 - \exp(-y^+/A^+)\right]$$

In the above expression,

$$y^+ = y\sqrt{\tau_0 \rho_0}/\mu_0,$$

$$\tau_0 = \mu_0 \frac{\partial u}{\partial y}\Big|_0$$ where the subscript o means that the quantity is evaluated at the wall, K = 0.41, and A^+ = 25 (Reference No. 8).

b) To express the quantity, $(\frac{\lambda}{c_p})_{eff}$ one defines a turbulent heat conduction in parallel with Fourier's law of heat conduction

$$q_t = -A_q c_p \Delta T, \qquad A_q = \lambda_t / c_p$$

Then one may form an effective heat conduction as

$$q_{eff} = q_0 + q_t = -c_p(\frac{\lambda}{c_p} + A_q)\nabla T = -c_p(\frac{\lambda}{c_p})_{eff}\nabla T$$

By defining a turbulent Prandtl number as

$$P_{rt} = A_\tau / A_q,$$

it can be shown that

$$(\frac{\lambda}{c_p})_{eff} = \frac{\mu}{P_r} + \frac{\rho \varepsilon_M}{P_{rt}}$$

The above equation governs the heat transport coefficients in the energy balance equation. P_r = 0.7 and P_{rt} = 1.0 are frequently assumed[8,9].

c) To express the quantity, $(\rho D)_{eff}$, it is assumed that, for both laminar and turbulent flows, Lewis number is equal to 1 as frequently the practice[10], i.e.

$$Le_{l,t} = (\frac{\lambda}{c_p} / \rho D)_{l,t} = 1$$

Then,

$$(\rho D)_{eff} = (\rho D)_l + (\rho D)_t = (\frac{\lambda}{c_p})_l + (\frac{\lambda}{c_p})_t = (\frac{\lambda}{c_p})_{eff}$$

F. Reaction Models

A one step forward overall gas phase reaction of second order is taken to represent the chemistry:

$C_3H_8 + 5O_2 + 5aH_2 \longrightarrow 4H_2O + 3CO_2 + 5aH_2$ where a is the molar ratio.

(a) Laminar reaction rate

To complete the species equation,

$$\hat{\omega} = F\rho^2 Y_F Y_O \exp(-E/RT)$$

where F is the pre-exponential constant: p, pressure; Y_F & Y_O, the species concentrations of fuel and oxidizer; E, activation energy; and R, the gas constant.

In the initial results discussed in Section III only laminar reaction rate is used.

(b) Turbulent reaction rate

The eddy-break-up model[11] for the turbulent flame is used as follows.

First, the reactedness of the gas, τ , is defined as

$$\tau = \frac{Y_F - Y_{F,u}}{Y_{F,b} - Y_{F,u}} = \frac{T - T_u}{T_b - T_u}$$

Then the time-mean volumetric rate of fuel consumption may be expressed as

$$\dot{\omega}_F = \left\{ (\tau \dot{Y}_{F,max})^{-1} + [C(1-\tau)\rho|\frac{\partial u}{\partial y}|]^{-1} \right\}^{-1}$$

where

$$\dot{Y}_{F,max} = F\rho^2 (\frac{a}{F}) Y_{F,max}^2 \exp(-E/RT_{max})$$

$$T_{max} = \frac{E}{4R}\left[-1 + \sqrt{1 + 8RT_f/E}\right]$$

$\frac{a}{f}$ = air fuel mass ratio

t_f = flame temperature

p = pressure

c = 0.35

In this model, the local reaction rate is taken to depend not only on a bimolecular Arrenious expression but also on the rate of break-up of the eddies by the action of turbulence.

G. Viscosity

A simple power law[9] is used.

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{0.625}$$

where $\mu_0 = 1.6758 \times 10^{-5}$ Kg/m·sec

$T_0 = 273.3$ °K

III. Finite Difference Solution of the Governing Equations

A. Coordinates and Grid Distribution

A rectangular field of 4.374cm x 1.413cm is imposed on the main region of the flow field shown in Fig. 1. In both x- and y-directions, uniform fine grid lines prevail over the interested region centered on the established flame front. Far away from the flame front, i.e. outside of the interest4e region, the grid lines follow a geometric series with the exception of the first and second grid lines near the boundary.

The magnitude of grid space (space between grid lines) is crucial to the proper propagation of the flame. It should be a fraction of the flame thickness which can be estimated by the thermal diffusivity divided by the reference flow velocity.

In the program, Δx is chosen to be 0.1 mm in the interested region resulting in a grid field of 93 x 31 points.

B. Control Volume

Figure 2 shows a grid point and its control volume. The arrangement is based on the work of Patankar and Spalding.[12]

The control volume, indicated by the dashed lines, is the region traversed by a rectangle of sides Δx and Δy. The area of the control surface normal to the x-direction is simply Δy since a unit thickness is assumed everywhere in the two dimensional region. The surface normal to the x-direction and located at e is midway between p and E. As a result p is not always the mid-point of e and w.

With the above arrangment a staggered grid which is similar to the one used by Harlow et. al.[13] is then used. It has the convenient feature that the velocity components, u and v, are stored at just the points at which they are needed for the calculation of the convective contribution to the balance of the quantity of question.

A finite difference equation for a node P is calculated by integrating the differential equation over the control volume indicated in the above. For evaluating the convection and diffusion fluxes through a control volume surface the arithmetic mean of the property values on either side of that face is taken. For other purposes a step-wise variation with discontinuties at the control volume surfaces is assumed.

C. Modifications to Finite Difference Equations

To ensure that the difference equations behave realistically when the particular method of computation leads to physically unreasonable results, the high-lateral-flux modification[14] is used. Under-relaxation is also used to ensure proper convergence of the solution.

D. Solution of the Finite-Difference Equations by TDMA

The finite-difference equations are solved by the successive use of the tri-diagonal matrix algorithm in the x and y directions.[12] The TDMA used is similar to the one developed by Roache.[15] The interior-point equation is written as

$$-A_i w_{i+1} + D_i w_i - B_i w_{i-1} = C_i , \qquad i = 1, M$$

The solution is of the following form

$$w_i = A_i' w_{i+1} + B_i'$$

where

$$A_i' = \frac{A_i}{D_i - B_i A_{i-1}'}$$

and

$$B_i' = \frac{C_i + B_{i-1}' B_i}{D_i - B_i A_{i-1}'}$$

For the left-hand boundary condition, one use:

(a) Dirichlet condition

$$A_i' = 0$$

$$B_i' = W_1$$

(b) Neumann condition

$$A_i' = 1$$

$$B_i' = 0$$

For the right-hand boundary condition,

(a) Dirichlet condition

$$W_M = a_M$$

(b) Neumann condition

$$W_M = B'_{M-1} / (1-A'_{M-1})$$

IV. Results and Discussion

The values of various parameters in the numerical computation are listed in Table 1. The programs were run on IBM 3033 at Princeton University Computer Center.

It is assumed that the steady stream on the flat plate in Figure 1 is a stoichiometric methane - air mixture under atmospheric pressure and temperature. Using Prandtl mixing length for the eddy diffusivity for momentum and using the bi-molecular Arrhenius expression for the chemical reaction the program was run for various upstream velocities to determine approximately the maximum flow velocity beyond which a flame, which is initiated by the hot segment (at 2000 °K) on the plate, would not propagate upstream. It was found that at a critical upstream speed of 1.8 m/s, the flame propagated upstream and that at 1.9 m/s the flame remains stationary. This compares with the experimental result of Gross[5] who reported that flash-backs occurred around a flow speed of 3 m/s using propane-air gas mixture over an airfoil plate. The critical upstream speed in the present program is expected to increase if eddy-break-up reaction model is used.

Figure 3 shows the flame envelope and typical velocity, temperature and concentration profiles at x = 2.2 cm for an upstream speed of 1.9 m/s. At the entrance (far upstream) it is

at one atmospheric pressure of 101.325 N/m^2 while at the exit (Far down-stream) 101.189 KN/m^2. Near the upper boundary the fuel concentration approaches to the up-stream value and the velocity exceeds the up-stream value by about 10%. The temperature profile shows a maximum in the middle but returns to the fixed wall temperature of 2000°K on the plate on the one side and approaches the up-stream temperature on the other.

To reach a steady state from a given set of initial profiles such as the one in the above 40 time steps (t=0.1 sec) and 1 minute and 35 seconds of computer time are needed to run the program.

The eddy-break-up reaction model has yet to be incorporated into the program and a series of paramatric studies need to be conducted.

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Table 1

Numerical Values Used in the Program

Parameter	Numerical Value
A+ (Defined in Section II.E.(a))	25
C_p Specific Heat	265 cal/Kg-^oK
E Activation energy	40000 cal/mole
K (Defined in Section II.E.(a))	0.41
Le Lewis no.	1
Pr Prandtl no.	0.7
Prt Prandtl no. for turbulent flow	1.0
Q Heat of combustion	1.1062×10^7 cal/Kg
R Gas constant for air	286.8 N-M/Kg-^oK
T_B Temperature of burned gas	2000^oK
T_U Temperature of unburned gas	300^oK
$Y_{f,u}$ Fuel concentration in the upstream	0.0594
Z Pre-exponential constant	0.5

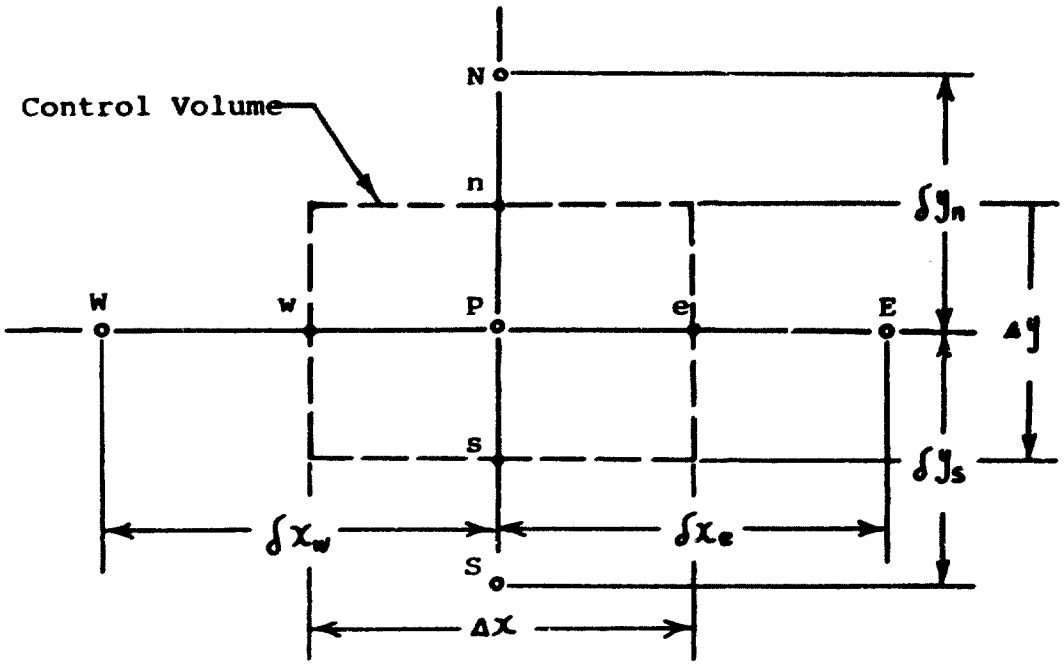

Figure 2 Control Volume

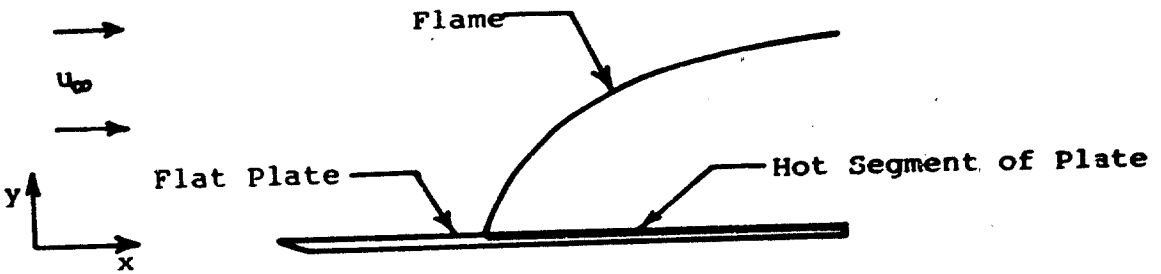

Figure 1 Schematic Diagram of a Flame on a Flat Plate

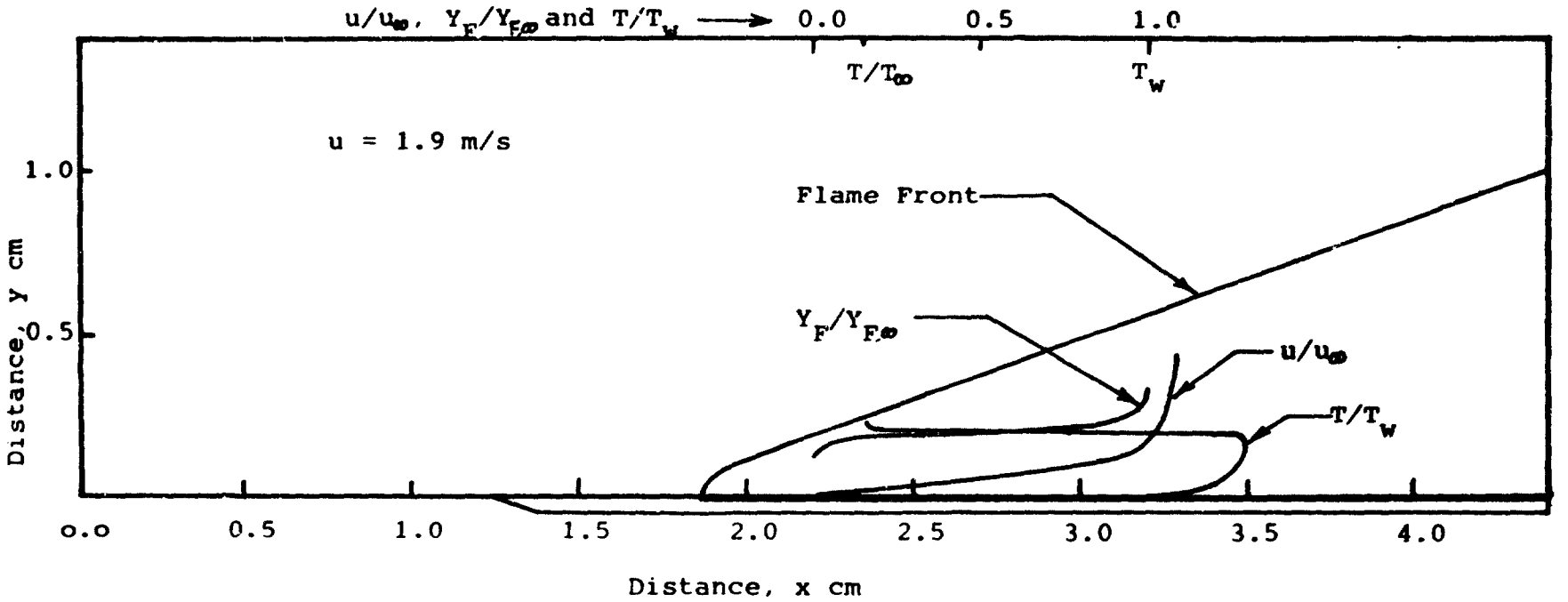

Figure 3 Steady Flame Attached on a Flat Plate