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EFFECT OF THERMAL EXPANSION ON THE STABILITY
OF TWO-REACTANT FLAMES

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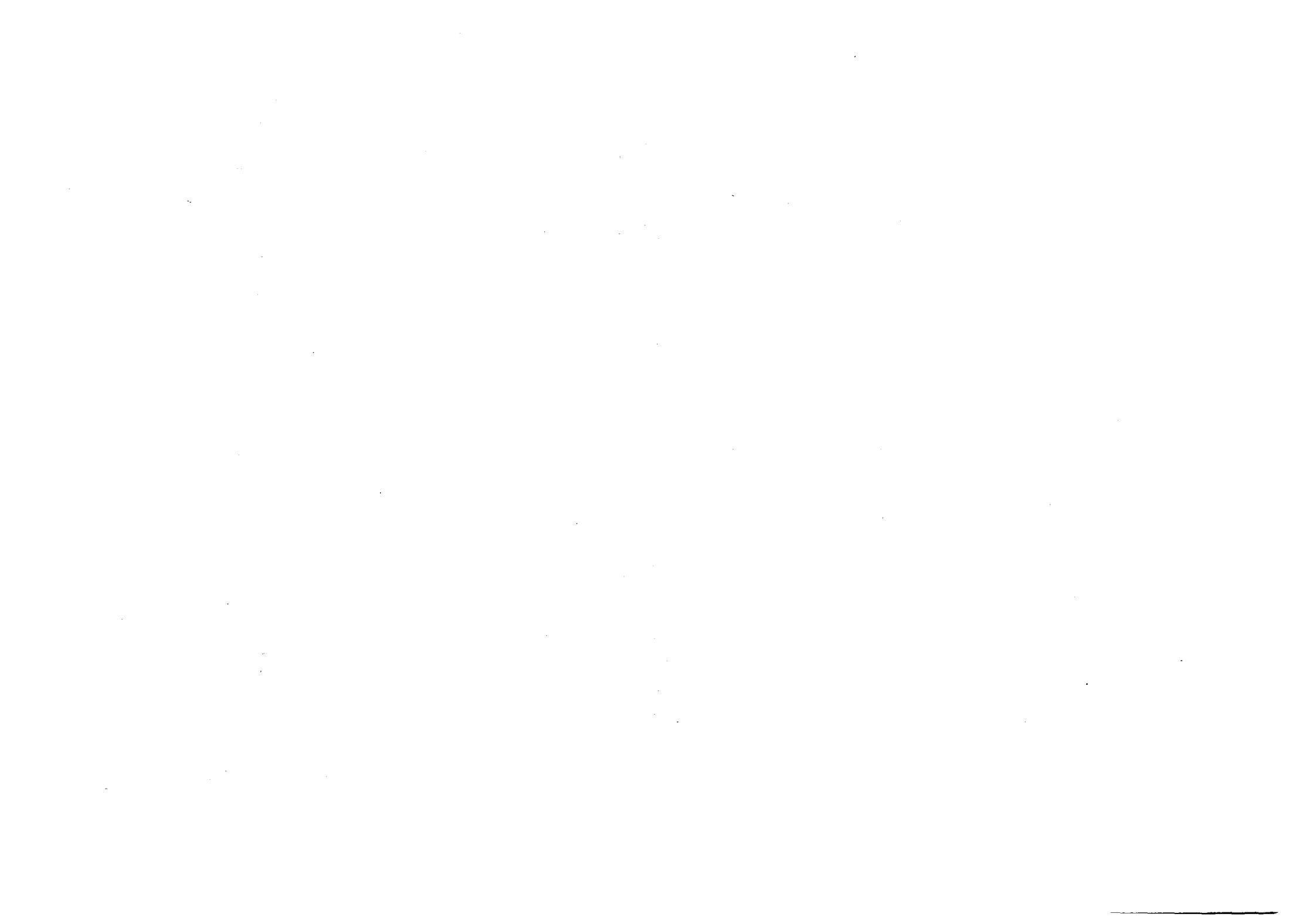
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Abstract

The full problem of flame stability for the two-reactant model, which takes into account thermal expansion effects for all disturbance wave lengths, is examined. It is found that the stability problem for the class of two-reactant flames is equivalent to the stability problem for the class of one-reactant flames with an appropriate interpretation of Lewis numbers.

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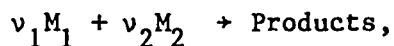


1. **Introduction.** Recently, Jackson and Kapila (1984, 1986a,b) reexamined the problem of the stability of a plane, premixed flame in the near-equidiffusional (NEF) framework. The study was aimed at understanding the role of thermal expansion on flame behavior. Neutral stability curves were obtained in the Lewis number-wave number plane and contrasted with the classical results of Sivashinsky (1977), who had employed the Constant Density Approximation (CDA).

The analysis was based on the simple kinetic model $A \rightarrow B$ which, as is well known, is also appropriate for a multi-reactant system when a single, deficient component controls the combustion process. Near stoichiometry, however, revisions are necessary since the number of controlling reactants is more than one. The first effort in this direction was due to Sivashinsky (1980) who examined the stability of a two-reactant model at EXACT stoichiometry, under the CDA; Joulin and Mitani (1981) later extended the result to near-stoichiometric mixtures. The essential point made by these studies is that the single-reactant results hold even near stoichiometry, provided the Lewis number is replaced by a suitably defined effective value.

The purpose of this note is to show that even when the CDA is abandoned and thermal expansion fully taken into account, the notion of an effective Lewis number persists. Thus, upon suitable interpretation, the results of Jackson and Kapila (1984, 1986a,b) can be applied to two-reactant systems.

2. **Governing Equations.** Consider the two-reactant model



where M_1 and M_2 denotes the chemical symbols of the deficient and abundant reactants respectively. Here ν_j is the stoichiometric coefficient for species j . We take the reaction to be irreversible and of Arrhenius-type so that its rate expression is of the form

$$(2.1) \quad \omega = B \rho^2 Y_1^m Y_2^n \exp(-E/RT),$$

where ρ is the density, Y_1 and Y_2 are the mass fractions of the deficient and abundant components, respectively, and T the temperature. The parameters appearing in the rate expression are the activation energy E , the universal gas constant R , the pre-exponential factor B , and the reaction orders m and n with respect to the deficient and abundant reactants, respectively.

The basic equations of the two-reactant system can be modelled by the following equations:

$$(2.2) \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0, \quad P = \frac{\rho RT}{W},$$

$$(2.3) \quad \rho \frac{D\mathbf{v}}{Dt} + \nabla P = \mu \left\{ \frac{1}{3} \nabla(\nabla \cdot \mathbf{v}) + \nabla^2 \mathbf{v} \right\},$$

$$(2.4) \quad \rho C_p \frac{DT}{Dt} - \frac{DP}{Dt} = \lambda \nabla^2 T + Q\omega,$$

$$(2.5) \quad \rho \frac{DY_j}{Dt} = \rho D_j \nabla^2 Y_j - \nu_j W_j \omega, \quad j = 1, 2.$$

Besides Y_j and T , the state of the system is determined by the density ρ , pressure P and velocity \mathbf{v} . The other quantities appearing above are the specific heat at constant pressure C_p , viscosity μ , thermal conductivity

λ , species diffusion coefficient D_j of species j , chemical heat release Q , molecular weight W_j of species j and molecular weight W of the inert. Finally, D/DT denotes the material derivative, defined by

$$(2.6) \quad \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \underset{\sim}{v} \cdot \nabla .$$

Equations (2.1) - (2.5) are supplemental by appropriate boundary conditions and jump conditions across the reaction zone.

For nondimensionalization of the governing equations, the state of the fresh mixture is chosen as the reference, defined by the constant values P_0 , ρ_0 , T_0 and v_0 , while the initial concentrations are rendered dimensionless relative to the initial concentration of the deficient reactant Y_{10} . The characteristic length and time scales are taken to be the adiabatic diffusion scales

$$(2.7) \quad l_0 = \lambda / (\rho_0 C_p v_0) , \quad t_0 = \lambda / (\rho_0 C_p v_0^2) .$$

It is convenient to introduce the flame Mach number as $M_0 = v_0 / c_0$, where c_0 is the frozen sound speed in the fresh mixture. Finally, pressure deviations from the ambient are referred to $\gamma M_0^2 P_0$, γ being the specific-heats ratio. The governing equations then take the dimensionless form

$$(2.8) \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \underset{\sim}{v} = 0 , \quad 1 = \rho T ,$$

$$(2.9) \quad \rho \frac{D\underset{\sim}{v}}{Dt} + \nabla P = Pr \left\{ \frac{1}{3} \nabla (\nabla \cdot \underset{\sim}{v}) + \nabla^2 \underset{\sim}{v} \right\} ,$$

$$(2.10) \quad \rho \frac{DT}{Dt} = \nabla^2 T + \alpha \Omega ,$$

$$(2.11) \quad \rho \frac{DY_j}{Dt} = L_j^{-1} \nabla^2 Y_j - \alpha_j \Omega, \quad j = 1, 2,$$

$$(2.12) \quad \Omega = \frac{D}{M_o^2} v_1 W_1 \rho_o Y_{10}^{m+n-1} \rho Y_1^m Y_2^n e^{-\theta/T}.$$

The yet undefined nondimensional parameters appearing above are:

$Pr = \mu C_p / \lambda$	Prandtl number,
$\alpha = QY_{10} / C_p T_o v_1 W_1$	Heat release number,
$\theta = E/RT_o$	Activation energy,
$\epsilon = (1 + \alpha)^2 / \theta$	Reciprocal activation energy,
$L_j = \lambda / \rho D_j C_p$	Lewis number for species j,
$D = \lambda B / \rho_o C_p c_o^2$	Damkohler number,
$\alpha_j = v_j W_j / v_1 W_1$	Parameter involving stoichiometry.

When a steady, planar, adiabatic flame is analyzed in the limit $\theta \rightarrow \infty$, i.e., $\epsilon \rightarrow 0$, the following expression for the Mach number M_o is obtained (see, e.g., Sen and Ludford (1979) and Mitani (1980)):

$$(2.13) \quad \frac{D}{M_o^2} = \frac{\alpha^{m+n+1} (1+\alpha)^2}{2 \alpha_2^n G(m,n,A)} \frac{\epsilon^{-1-m-n} Y_{10}^{1-m-n}}{v_1 W_1 \rho_o L_1^m L_2^n} e^{\frac{\theta}{1+\alpha}} \{1 + O(\epsilon)\},$$

where

$$(2.14) \quad G(m,n,A) = \int_0^\infty \xi^m (\xi+A)^n e^{-\xi} d\xi.$$

Here, A is the normalized final concentration of the abundant, given by

$$(2.15) \quad A = \frac{\alpha}{\epsilon L_2} (\phi - 1)$$

and ϕ is the equivalence ratio ($v_1 W_1 Y_{20} / v_2 W_2 Y_{10}$). Equation (2.13) is valid for the entire range of mixture ratio. However, we are only interested in the

mixture-ratio range $\phi - 1 = O(\epsilon)$; i.e., near-stoichiometric mixtures, since the reaction rates are then governed by the deficient component as well as the abundant component of the mixture. The special cases of very-near stoichiometry ($\phi - 1 = O(\epsilon^2)$; i.e., $A \rightarrow 0$) and away-from stoichiometry ($\phi - 1 = O(1)$; i.e., $A \rightarrow \infty$) can be considered as limiting cases of the near-stoichiometric analysis, and will be discussed in the conclusions. Equation (2.13) also shows that the Mach number is exponentially small in the limit of large activation energy.

The near-equidiffusional formulation (NEF), in addition to large activation energy, is characterized by near-unity Lewis numbers and nearly-uniform enthalpies, i.e.,

$$(2.16) \quad L_1^{-1} = 1 - \epsilon \left(\frac{\ell_1}{\alpha}\right), \quad T + \alpha Y_1 \equiv H = 1 + \alpha + \epsilon h,$$

$$(2.17) \quad L_2^{-1} = 1 - \epsilon \left(\frac{\ell_2}{\alpha}\right), \quad T + \frac{\alpha}{\alpha_2} Y_2 \equiv G = 1 + \frac{\alpha}{\alpha_2} Y_{2f} + \epsilon g.$$

Here, $Y_{2f} = Y_{20}/Y_{10}$ denotes the dimensionless mass fraction of Y_2 in the fresh mixture. Then, to leading order in ϵ , equations (2.8), (2.9) remains unaltered, while equations (2.10) and (2.11) are replaced by

$$(2.18a) \quad \rho \frac{DT}{Dt} - \nabla^2 T = 0 \quad \text{in the burnt region,}$$

$$(2.18b) \quad T = 1 + \alpha \quad \text{in the unburnt region,}$$

$$(2.19a) \quad \rho \frac{Dh}{Dt} = \nabla^2 h + \left(\frac{\ell_1}{\alpha}\right) \nabla^2 T,$$

$$(2.19b) \quad \rho \frac{Dg}{Dt} = \nabla^2 g + \left(\frac{\ell_2}{\alpha}\right) \nabla^2 T.$$

Equations (2.8), (2.9), (2.18) and (2.19) now constitute the basic set.

The following analysis is by now standard, and the reader is referred to Jackson and Kapila (1984) for details, hereafter referred to as I. For a two-dimensional flow, let the reaction-zone location be given by $x = x_f \equiv F(y,t)$. It is convenient to shift to a reference frame in which the reaction zone is stationary. Let a new coordinate ξ be defined by the transformation

$$(2.20) \quad x = F(y,t) + \xi ,$$

and let the unburnt and burnt regions be confined, respectively, to $\xi < 0$ and $\xi > 0$. Then one obtains equations (8)-(22) of I, except now the enthalpy equation (14I) is replaced by the enthalpy equations for h and g ,

$$(2.21a) \quad \rho (h_t + Sh_\xi + vh_y) = \nabla^2 h + \left(\frac{l_1}{\alpha}\right) \nabla^2 T,$$

$$(2.21b) \quad \rho (g_t + Sg_\xi + vg_y) = \nabla^2 g + \left(\frac{l_2}{\alpha}\right) \nabla^2 T,$$

while the boundary conditions (21I) and (22I) at $\xi = 0$ are replaced, respectively, by

$$(2.22) \quad \delta T_\xi = \frac{-\alpha e^{h/2}}{\sqrt{(1+F_y^2)} G(m,n,A)} \left\{ \int_0^\infty \xi^m (A+g-h+\xi)^n e^{-\xi} d\xi \right\}^{1/2},$$

$$(2.23) \quad \delta h_\xi = - \left(\frac{l_1}{\alpha}\right) \delta T_\xi , \quad \delta g_\xi = - \left(\frac{l_2}{\alpha}\right) \delta T_\xi .$$

Equations (8I)-(22I), together with (2.21)-(2.23) describe completely the NEF problem.

3. **Linearization.** Small perturbations of the steady flame are governed by linearized equations, which can be obtained by setting

$$(3.1) \quad \psi = \psi^S(\xi) + \sigma \bar{\psi}(\xi, y, t)$$

for all variables and taking the limit $\sigma \rightarrow 0$. We focus our attention only on the enthalpy equations (2.21) and the boundary conditions (2.22) and (2.23) since linearization of the other equations yields the identical equations of I.

Linearization of (2.21) leads to

$$(3.2a) \quad \rho^S \bar{h}_t + \bar{h}_\xi + \bar{m} h_\xi^S = \bar{h}_{\xi\xi} + \bar{h}_{yy} - \bar{F}_{yy} h_\xi^S \\ + \left(\frac{\ell_1}{\alpha}\right) (\bar{T}_{\xi\xi} + \bar{T}_{yy} - \bar{F}_{yy} T_\xi^S),$$

$$(3.2b) \quad \rho^S \bar{g}_t + \bar{g}_\xi + \bar{m} g_\xi^S = \bar{g}_{\xi\xi} + \bar{g}_{yy} - \bar{F}_{yy} g_\xi^S \\ + \left(\frac{\ell_2}{\alpha}\right) (\bar{T}_{\xi\xi} + \bar{T}_{yy} - \bar{F}_{yy} T_\xi^S)$$

for \bar{h} and \bar{g} , respectively, while linearization of the jump conditions (2.22) and (2.23) at $\xi = 0$ yields

$$(3.3) \quad \delta \bar{T}_\xi = -\frac{\alpha}{2} \{ \bar{h} + H(\bar{g} - \bar{h}) \},$$

$$(3.4) \quad \delta \bar{h}_\xi = -\left(\frac{\ell_1}{\alpha}\right) \delta \bar{T}_\xi, \quad \delta \bar{g}_\xi = -\left(\frac{\ell_2}{\alpha}\right) \delta \bar{T}_\xi.$$

Here,

$$(3.5) \quad H = n \frac{G(m, n-1, A)}{G(m, n, A)} .$$

If we define a new function \bar{f} by

$$(3.6) \quad \bar{f} = \bar{h} + H (\bar{g} - \bar{h}),$$

then (3.2) reduces to a single equation for \bar{f} , namely

$$(3.7) \quad \rho^s \bar{f}_t + \bar{f}_\xi + \bar{m} f_\xi^s = \bar{f}_{\xi\xi} + \bar{f}_{yy} - \bar{F}_{yy} f_\xi^s \\ + \frac{1}{\alpha} (\ell_1 + H (\ell_2 - \ell_1)) \{ \bar{T}_{\xi\xi} + \bar{T}_{yy} - \bar{F}_{yy} T_\xi^s \},$$

while (3.3) and (3.4) determines the jump conditions at $\xi = 0$,

$$(3.8) \quad \delta \bar{T}_\xi = -\frac{\alpha}{2} \bar{f}, \quad \delta \bar{f}_\xi = -\frac{1}{\alpha} (\ell_1 + H (\ell_2 - \ell_1)) \delta \bar{T}_\xi .$$

These equations are identical to the linearized enthalpy equation for the premixed flame (see (30I), (36I), and (42I)) with a reduced Lewis number ℓ_c , defined by

$$(3.9) \quad \ell_c = \ell_1 + H (\ell_2 - \ell_1) .$$

4. Discussion and Conclusions. The stability problem of the two-reactant flame consists of the linear system (24I)-(42I), with (30I) and (36I) replaced by (3.7), and the boundary condition (42I) replaced by (3.8). In particular, we find that this system is governed only by the parameter ℓ_c , defined in

(3.9). It is only here that the mixture ratio appears through H , and thus we consider the following three limiting cases. For near-stoichiometric mixtures, H is given by (3.5) and can not be simplified further. For very-near stoichiometry, H is given by

$$(4.1a) \quad H = \frac{n}{m+n} + 0(\epsilon) \quad , \quad \phi - 1 = 0 (\epsilon^2),$$

and the corresponding reduced Lewis number becomes

$$(4.1b) \quad l_c = \frac{m l_1 + n l_2}{m + n} + 0 (\epsilon),$$

i.e., the average value of the two Lewis numbers weighted by their respective reaction orders (Joulin and Mitani (1981)). Finally, away from stoichiometry, H is given by

$$(4.2a) \quad H = \frac{\epsilon n}{\alpha(\phi-1)} + 0 (\epsilon^2) \quad , \quad \phi - 1 = 0 (1),$$

with corresponding l_c ,

$$(4.2b) \quad l_c = l_1 + 0 (\epsilon).$$

Thus, for far-from stoichiometric mixtures, the stability problem reduces to that of a one-reactant flame governed by the Lewis number of the deficient component.

Sivashinsky (1980) and Joulin and Mitani (1981) have shown that within the diffusional-thermal model, the stability problem for two-reactant flames at or near stoichiometry reduces to the stability problem for single-reactant flames with a reduced Lewis number. We have shown that the above result also holds for the more important case when thermal expansion is accounted for, and for the entire range of mixture ratio. The following general statement can now be made: The linear stability problem for the class of two-reactant flames is equivalent to the stability problem for the class of one-reactant flames with Lewis number $L = 1 + \epsilon(\ell_c/\alpha)$. The effects of heat loss and gravity do not alter this conclusion.

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