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UNSTEADY PLANAR DIFFUSION FLAMES: IGNITION, TRAVEL, BURNOUT

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Introduction

Consider an impervious noncatalytic isothermal squat rectangular-solid container, with height significantly smaller than the length of a side of the square cross section [Fig.1(a)]. The container is taken to be filled initially with purely gaseous reactants, with the oxidizer separated from the fuel by a thin impervious planar diaphragm. Such a diaphragm might be formed by a stretched thin film of a hydrocarbon polymer such as parylene. For specificity, we take the upper half volume to be filled uniformly with oxygen diluted with helium, and the lower half volume to be filled uniformly with hydrogen diluted with argon, such that the two half volumes have equal pressure, temperature, density, and (hence) "average molecular weight". At time zero, with minimal disturbance, small perforations of the diaphragm are made at a multitude of sites, so that the contents of the upper and lower half volumes begin to interdiffuse. After a short interval of time, a layer, of thin but finite thickness and containing combustible mixture, is formed; the layer extends to each side of the midplane [Fig.1(b)]. Ignition of the combustible mixture results in a rapid laminar flame propagation through that portion of the container contents with mixture within the fuel-rich and fuel-lean flammability limits. For hydrogen and oxygen at roughly atmospheric pressure and ambient temperature, and not too far from stoichiometric proportion, such a flame propagation takes but a small fraction of a second to consume the combustible mixture, for a cross-section dimension of 10 cm or so. For a fuel-lean mixture, excess oxygen is available to convert the remnants of the diaphragm to purely gaseous products, so no soot forms. The result of the flame propagation is the formation of a vigorous planar diffusion flame at the interface between the hydrogen and oxygen [Fig.1(c)].

The narrow layer of hot combustion products will remain planar, and not rapidly disintegrate under buoyant instability (refs. 1, 2) into a convoluted pattern of adjacent "fingers" of relatively hot and cold gas, if the dimensionless Rayleigh number $Ra < O(2000)$, where by definition, $Ra \equiv [(\Delta T)/T_{ref}]\, g a^3/(\nu\kappa)$. Here, T_{ref} denotes a typical temperature and (ΔT), a characteristic temperature difference; g is the magnitude of the gravitational acceleration; a is a characteristic physical dimension along the direction of gravity; ν characterizes the kinematic viscosity of the gaseous medium and κ, the thermal diffusivity. For $(\Delta T)/T_{ref} \approx 8$, $(\nu\kappa) \approx 0.16$ cm^4/s^2, $g = g_o \approx 10^3$ cm/s^2, the typical dimension of an experimental apparatus is restricted to significantly less than one-quarter of a centimeter. (We do not want even to approach the critical Rayleigh number, because the idealizations adopted in applying the criterion are many.) This minute scale is entirely impractical, not only for diagnostic instrumentation, but also because heat losses to encompassing cold walls in such close proximity would quench the burning. However, in a microgravity environment (ref. 3) such that $g = 10^{-5}\, g_o$, the critical dimension $a \approx 10$ cm. Thus, in an apparatus of 5 cm in height, the fact that hot combustion products in the narrow burned layer lie below a colder, more dense oxygen/helium mixture should set off no symmetry-disrupting gravitational instability in a microgravity environment.

The upshot is that, in microgravity, a thin *planar* diffusion flame is created and thenceforth travels so that the flame is situated at all times at an interface at which the hydrogen and oxygen meet in stoichiometric proportion. If the initial amount of hydrogen is deficient relative to the initial amount of oxygen, then the planar flame will travel further and further into the half volume initially containing hydrogen [Fig.1(d)], until the hydrogen is (virtually) fully depleted. Of course, when the amount of residual hydrogen becomes small, the diffusion flame is neither vigorous nor thin; in practice, the flame is extinguished before the hydrogen is fully depleted, owing to the finite rate of the actual chemical-kinetic mechanism. The rate of travel of the hydrogen-air diffusion flame is much slower than the rate of laminar flame propagation through a hydrogen-air mixture. This slow travel facilitates diagnostic detection of the flame position as a function of time, but *the slow travel also means that the time to burnout (extinction) probably far exceeds the testing time (typically, a few seconds) available in earth-sited facilities for microgravity-environment experiments.*

We undertake an analysis to predict: (1) the position and temperature of the diffusion flame as a function of time; (2) the time at which extinction of the diffusion flame occurs; and (3) the thickness of quench layers formed on side walls (i.e., on lateral boundaries, with normal vectors parallel to the diffusion-flame plane), and whether, prior to extinction, water vapor formed by burning will condense on these cold walls.

Issues Under Investigation

The simplest reasonable theoretical model not only adopts the standard Shvab-Zeldovich simplifications (refs. 4, 5) (direct one-step irreversible chemical reaction, binary diffusion, uniformity in space and time of the average molecular weight of the gaseous mixture, simple variation of the molecular-transport coefficients with thermodynamic state, constancy of the ratio of any two molecular-transport coefficients, etc.); the model goes further, in the manner of Burke and Schumann (refs. 4, 5) to idealize the rate of chemical reaction as effectively infinitely rapid, relative to the rate of transport. (The ratio of the reaction rate to the flow rate is defined to be the first Damköhler number, and is denoted D_1.) The Burke-Schumann treatment is a *limiting* case in that only the rate of mixing, not the rate of reaction as well, impedes the rate of formation of product species. The limit is mathematically singular in that the flame is a Dirac-delta-function-type sink for reactant concentrations, and a source for product concentrations and heat: each of these thermodynamic state variables is continuous at the fuel-oxidizer interface, but each has first (and all higher) derivatives that are discontinuous at the interface. In the Burke-Schumann limit, the flame is an (in general, moving) boundary between fuel and oxidizer (refs. 6, 7), and the mathematical techniques usefully associated with the solution of Stefan problems (refs. 8, 9) may be applied in this aerothermochemical context. The Stefan-problem nature of diffusion-flame analyses is often obscured because attention is typically confined to steady scenarios, or at least to quasisteady scenarios in which the temporal dependence is approximated as parametric (and no explicit temporal derivatives are retained). The Stefan-problem nature of diffusion-flame analyses is obscured further because attention is usually confined to the special case of equal diffusion coefficients for all species and heat (and perhaps momentum as well). In this special case, the identity of convective-diffusive differential operators permits reformulation of the boundary/initial-value problem in terms of linear combinations of the dependent variables; the upshot is that the flame locus need be identified only *after* the formal solution is completed. In practice, the molecular diffusivities virtually always differ, and differ significantly for cases (such as the one cited here, involving hydrogen) in which the molecular weights of the major species differ significantly. In these cases, the time-varying position of the thin flame must be identified explicitly *during* the course of solution of the boundary/initial-value problem.

A hydrogen/oxygen diffusion flame, especially in the geometric simplicity afforded by microgravity, permits us, without the usual complicating need to account for the black-body radiation associated with soot, to test whether the Shvab-Zeldovich/Burke-Schumann formulation predicts experimentally observed behavior. In such a formulation, the ratio of the Fickian-diffusion coefficient for the fuel vapor, D_F, to the thermal diffusivity, κ--denoted as one Lewis-Semenov number, Le_F, and the ratio of the Fickian-diffusion coefficient for oxidizer, D_O, to the thermal diffusivity, κ--denoted as another Lewis-Semenov number, Le_F, are taken to be constant in space and time. (These convenient definitions are the inverse of the conventional definitions for Lewis-Semenov numbers.) In practice, the ratios vary in space and time within the flow, despite the fact that, in the *initial* configuration, we have diluted hydrogen with argon, and oxygen with helium, so that the average molecular weight is everywhere the same. We hope that the empirical assignment of optimal values for the Lewis-Semenov numbers, Le_F, and Le_ϕ, will permit us to fit some of the microgravity data (explicitly, the position and temperature at the thin flame in some of the experiments). We further hope that the guidance from that experience will permit us to assign values to the Lewis-Semenov numbers to predict the corresponding observations in the remainder of the experiments. If so, the viability of the simple Shvab-Zeldovich/Burke-Schumann model to quantify, to a practically useful accuracy, key properties in a difficult-to-analyze diffusion flame will have been demonstrated.

The scenario in Fig.1 affords many simplifications beyond a modest role for radiative heat transfer. There is no "nitrogen chemistry", and no gasification of an initially condensed-phase fuel, to add complication. We expect no cellular behavior, which is associated with flame-scale instabilities in premixed flames, and which is typically not observed for modest-scale, vigorous diffusion flames. Aside from quenching near the cold lateral surface of the container, we are examining unsteady, planar phenomena, for which analysis can be carried out entirely in terms of a convenient Lagrangian coordinate; such is not the case for spherical symmetry. Away from the quench layers, the only significant velocity component is perpendicular to the plane of the flame; hence, the problem is distinct from the counterflow, in which velocity components perpendicular and parallel to the plane of the diffusion flame arise.

Diffusion-Flame Extinction

By singular-perturbational analysis, it is possible to perturb about the Burke-Schumann limit (rate of reactant conversion limited by diffusive transport only), and to calculate when the conditions in a burn are sufficient for extinction, according to a direct one-step irreversible second-order large-Arrhenius-activation-temperature model of the finite-rate chemical kinetics. This sufficiency criterion is the consequence of the nonuniqueness of the solution to the formulation of steady burning in systems with separated "feeds" of fuel and oxidizer, for kinetics of the genre just described. Because, at extinction, kinetic effects are limited to a narrow quasisteady zone of reactant interpenetration (roughly) centered about the thin-flame site, we are able to apply, to our unsteady one-dimensional diffusion flame, the sufficient condition for extinction originally derived for a steady two-dimensional counterflow-type diffusion flame (refs. 10, 11). The sufficient condition for extinction amounts to identifying an explicit limiting value for the first Damkohler number, $(D_1)_\ell$, for a fixed set of other flow parameters. The checking for satisfaction of this explicit criterion for extinction may be facilely and rapidly carried out at each time step, as a peripheral calculation to the Shvab-Zeldovich/Burke-Schumann analysis. Indeed, paradoxically, owing to the singular-perturbation basis by which the sufficiency condition for extinction is derived, it is convenient to apply the criterion only if we have available the results for a Shvab-Zeldovich/Burke-Schumann analysis of the scenario of Fig.1(d). If we simply adopt any reasonable finite-rate chemical-kinetic model and compute the predicted aerothermochemical evolution from the initial configuration, then, while we may try to infer when extinction occurs according to some intuitive criterion, no explicit sufficiency criterion for extinction is available. Thus, the availability of a solution in the Burke-Schumann limit not only affords a lowest-order estimate of the time to extinction based on total exhaustion of the deficient reactant; the solution is also a first step in obtaining a finite-reaction-rate-based upgrade of the lowest-order estimate of the time to extinction.

What Related Experiment Is Feasible in Earth Gravity?

Suppose the contents of the container in Figure 1(a) are altered to be stably stratified, so that relatively light gas lies over relatively heavy gas; explicitly, suppose the upper half-volume initially contains hydrogen diluted with helium, and the lower half-volume initially contains oxygen diluted with argon. (The motivation for the dilution is to avoid so hot a flame that complications arise, from dissociation of product species, from enhanced hot-gas radiation, and/or from thermal threat to the integrity of the container.) After ignition for fuel-deficient test conditions, the hot product species would be dominantly water vapor. The molecular weight of this species is much greater than that of hydrogen or helium, and much less than that of oxygen or argon. Thus, at least until diffusion permits argon significantly to enter the hydrogen-containing subdomain, and helium significantly to enter the oxygen-containing subdomain, there seems the possibility that the stabilizing stratification based on species-concentration profiles might override the destabilizing stratification based on thermal (hot-under-cold) considerations. Of course, the relative contributions to the density stratification along the (vertical) direction of the earth-gravity acceleration would determine whether the flame is stable. However, the alternative initial stratification described in this paragraph is not consistent with conditions amenable to Shvab-Zeldovich/Burke-Schumann modeling. Simplistic Shvab-Zeldovich modeling is expected to pertain only to those conditions in which the average molecular weight is at least roughly uniform at all sites in the container for all times of interest, and such is clearly not the case for the alternative initial stratification. A more meticulous theoretical treatment (e.g., of the equation of state) would be suitable for the alternatively stratified scenario--so the scenario lies outside the scope of our first objectives.

Accordingly, in this project, we confine attention to the scenarios depicted in Figure 1. Testing in the NASA Lewis Research Center drop tower with a two-seconds-duration microgravity environment is to be carried out during the summer of 1994. The objective is to demonstrate that we can achieve a planar diffusion flame, upon breaking the thin-film separator and igniting, probably by use of a hot wire. However, the available two-second testing time is exhausted before the flame has undergone virtually any translation. As we noted earlier, data collection must be deferred until testing is carried out in the prolonged microgravity environment available in space flight. In that prolonged microgravity environment, we anticipating measuring, as functions of time since ignition: the flame temperature and position (including the time of flame extinction); the sidewall-quench-layer thickness; the chamber pressure; and the heat transfer at each end wall and at multiple sites along one side wall. We also plan to measure the total hydrogen, oxygen, and water substance in the chamber at the time of extinction. For a given set of parameter assignments, the previously described model can be used to try to predict the observations. Whether accurate predictions are accessible via such a simplistic model, or whether the model is limited to diagnostic use (in that empirical assignment of the Lewis-Semenov numbers remains requisite to recovering the observations) awaits the availability of data.

Examples of Model Prediction

For the fuel-lean or stoichiometric systems of hydrogen/argon initially segregated from oxygen/helium (Figure 1), the one-step irreversible reaction $2\,H_2 + O_2 \rightarrow 2\,H_2O$ - Q (heat) implies that the stoichiometrically adjusted mass fraction for fuel $F \equiv 9\,\tilde{Y}_{H_2}$, and that for oxidizer $\phi \equiv (9/8)\ \tilde{Y}_{O_2}$, where $\tilde{Y}_j$ is the mass fraction of species j. If t denotes time since ignition; c_p and c_v, heat capacity at constant pressure and volume, respectively; p, pressure; ρ, density; T, temperature; u, speed in the z direction; and subscript i, initial value, then we nondimensionalize as follows:

$$\bar{z} \equiv z/a, \text{where} -a \le z \le a,\ \ -1 \le \bar{z} \le 1;\ \ \tau \equiv \kappa_i t/a^2,\ \text{ where }\ t > 0;$$

$$\bar{T} \equiv T/T_i,\ \ \bar{p} \equiv p/p_i,\ \ \bar{\rho} \equiv \rho/\rho_i,\ \ \bar{u} \equiv u/\left(\kappa_i/a^2\right),\ \ \gamma \equiv c_p/c_v,\ \ D_2 \equiv Q/\left(36 c_p T_i\right)\ .$$

The dimensionless flame position is denoted $Z_f(\tau)$; a stagnation plane, $Z_s(\tau)$. The following set of values for the six dimensionless parameters arising in a Shvab-Zeldovich/Burke-Schumann formulation for the "core" flow (i.e., ignoring side-wall quench layer) is termed nominal:

$$Le_F = 1.78,\ \ Le_\phi = 0.432,\ \ F_i = 0.914,\ \ \phi_i = 0.914,\ \ D_2 = 17.9,\ \ \gamma = 1.4\ .$$

Sample results in the dimensionless physical coordinate $\bar{z}$ (obtained by Crank-Nicholson integration, after transformation to "boundary-fixing" Lagrangian coordinates) are presented in Figures 2-6. With the anticipated availability of data from experiments in microgravity, we may ascertain what (if any) assignment of the Lewis-Semenov numbers permits this simplistic, convenient model to recover key combustion behavior, such as flame translation and flame temperature as functions of time.

Acknowledgments

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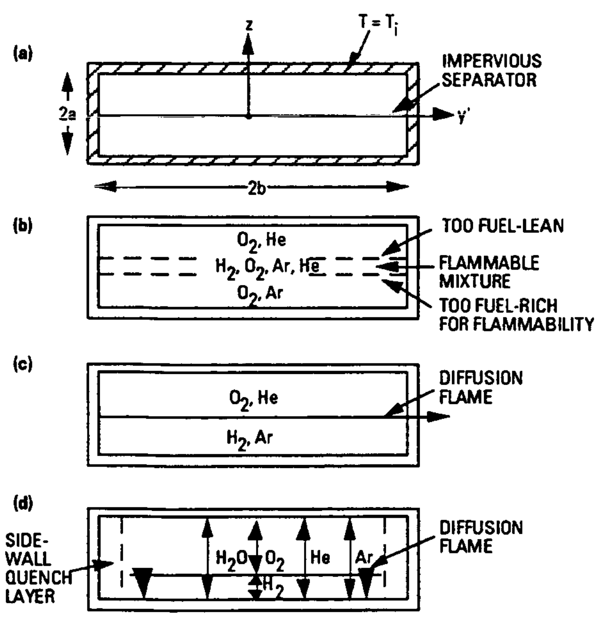

Figure 1. Geometry for a planar translating diffusion flame: (a) argon-diluted hydrogen, initially separated from helium-diluted oxygen, by a thin film, the contents of each half-volume V being at, pressure p_i, density ρ_i, and temperature T_i; (b) incipient interdiffusion of reactants after perforation of the separator; (c) diffusion flame, after ignition and deflagration of the narrow combustible layer; and (d) subsequent travel of the diffusion flame for a hydrogen-deficient scenario, with extinction near the lateral walls of the isolthermal container.

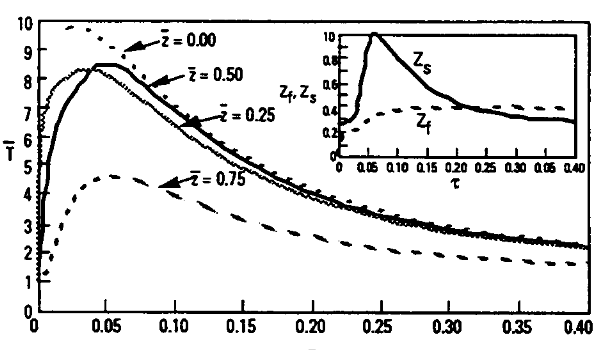

Figure 2. For nominal parametric values, the dimensionless temperature $\overline{T}$ vs. the dimensionless time τ, for four values of the dimensionless spatial coordinate $\bar{z}$. The inset presents the diffusion-flame position, $Z_f(\tau)$, and the stagnation-plane position, $Z_s(\tau)$, for the velocity $\bar{u}$.

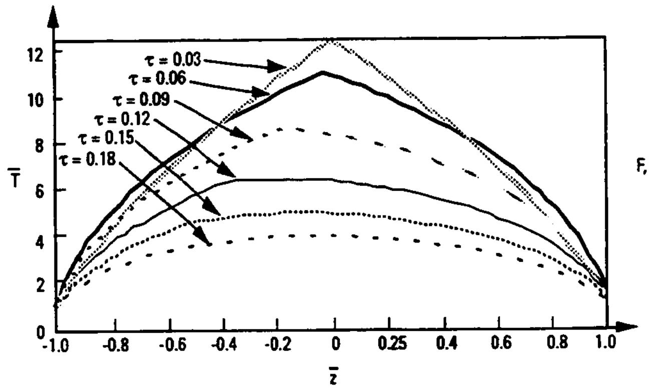

Figure 3. For the nominal case except $F_i/\phi_i = 0.5$, $\phi_i = 0.914$, $Le_F = 1.6$, and $Le_\phi = 0.4$, the dimensionless temperature $\overline{T}$ vs. the dimensionless coordinate $\bar{z}$, at several dimensionless times (since ignition) τ.

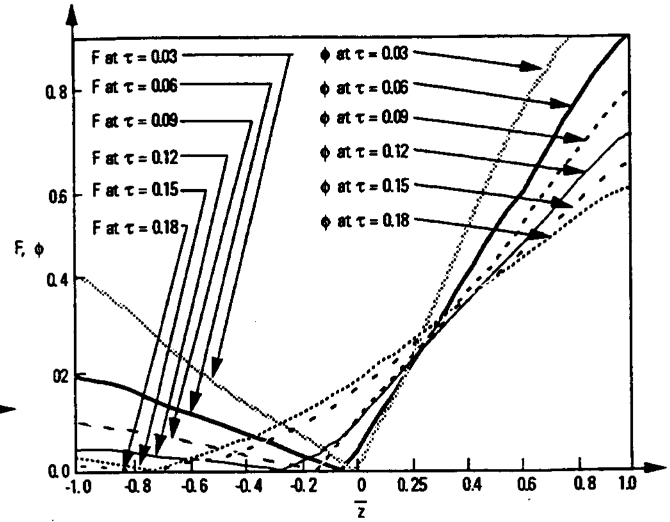

Figure 4. For the case of Figure 3, the stoichiometrically adjusted mass fraction for fuel F, and for oxidizer ϕ, vs. the dimensionless spatial coordinate $\bar{z}$, at several dimensionless times τ.

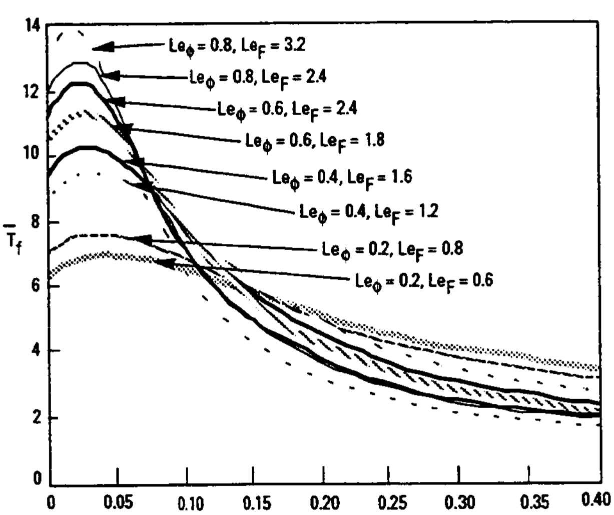

Figure 5. For the nominal case except for the values ascribed to the Lewis-Semenov numbers, Le_F and Le_ϕ, the dimensionless flame temperature $\overline{T}_f$ vs. the dimensionless time τ.

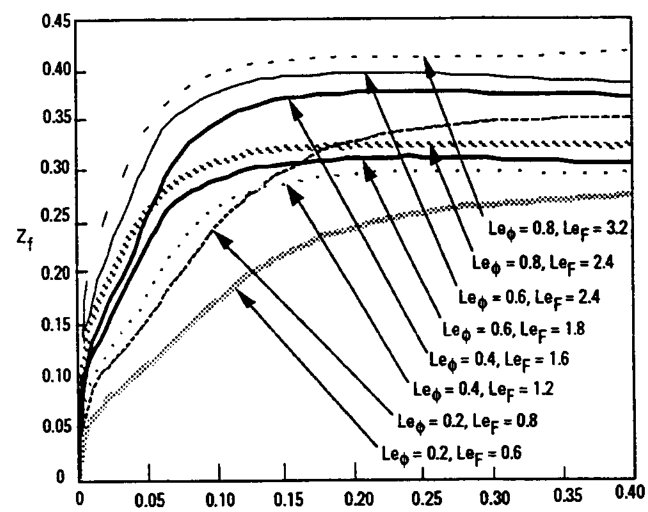

Figure 6. For the cases presented in Figure 5, the dimensionless flame position Z_f vs. the dimensionless time τ.