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NUMERICAL MODELING OF FLAME-BALLS IN FUEL-AIR MIXTURES

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Introduction

For over forty years it has been known that, as a result of buoyancy, the ignition of near limit hydrogen-air mixtures can lead to the formation of flame-caps–discrete curved flames which are small on the scale of the confinement vessel [1]. More recently it has been shown that at low gravity, when buoyancy effects are small, flame-balls can be generated [2]. These are stationary spherical structures whose existence appears to require a near-limit mixture, a small Lewis number and heat losses from radiation. It is our goal to combine computational modeling with existing experimental and theoretical studies (NASA) of these structures so that an improved understanding of flammability limits and near-limit phenomena will occur. The question of flammability limits is of fundamental importance and has long been examined. It is of great practical importance to predict, from first principles, a limit mixture strength that agrees with experimental values for the configuration at hand. Flame-balls provide an excellent configuration in which convective losses can be eliminated and the resulting stable solutions are produced from a diffusive, reactive and radiative balance.

Problem Formulation

Although analytical modeling provides convincing evidence that the key physical ingredients of flame-balls have been identified, quantitative confirmation can only come from detailed numerical simulations. Our goal is to predict theoretically the mass fractions of the species and the temperature as functions of the independent coordinate r. Upon neglecting viscous effects, body forces, and the diffusion of heat due to concentration gradients, the equations governing the structure of a steady, spherically symmetric, isobaric flame-ball are

$$-\frac{1}{r^2}\frac{d}{dr}(r^2\rho Y_k V_k) + \dot{\omega}_k W_k = 0, \qquad k = 1, 2, \ldots, K, \tag{1}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\lambda\frac{dT}{dr}\right) - \sum_{k=1}^{K}\rho Y_k V_k c_{p_k}\frac{dT}{dr} - \sum_{k=1}^{K}\dot{\omega}_k h_k W_k - \frac{1}{r^2}\frac{d}{dr}(r^2 q_R) = 0, \tag{2}$$

$$\rho = \frac{p\overline{W}}{RT}. \tag{3}$$

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In these equations r denotes the independent spatial coordinate; T, the temperature; Y_k, the mass fraction of the k^{th} species; p, the pressure; ρ, the mass density; W_k, the molecular weight of the k^{th} species; $\overline{W}$, the mean molecular weight of the mixture; R, the universal gas constant; λ, the thermal conductivity of the mixture; c_p, the constant pressure heat capacity of the mixture; c_{pk}, the constant pressure heat capacity of the k^{th} species; $\dot{\omega}_k$, the molar rate of production of the k^{th} species per unit volume; h_k, the specific enthalpy of the k^{th} species; q_R the radiative heat flux and V_k, the diffusion velocity of the k^{th} species.

Utilizing the kinetic theory of dilute gas mixtures, we can write the following expression for the species diffusion velocities

$$V_k = -\sum_{l=1}^{K} D_{kl} \nabla X_l - \theta_k \nabla \log(T), \tag{4}$$

where D_{kl}, $1 \leq k, l \leq K$, are the species diffusion coefficients and θ_k, $1 \leq k \leq K$, are the thermal diffusion coefficients. The species diffusion coefficients are symmetric and satisfy the important relations

$$\sum_{k=1}^{K} Y_k D_{kl} = 0, \; 1 \leq l \leq K, \qquad \sum_{k=1}^{K} Y_k \theta_k = 0, \tag{5}$$

which guarantee the mass conservation constraint

$$\sum_{k=1}^{K} Y_k V_k = 0. \tag{6}$$

Using the recent theory of iterative transport algorithms [3], rigorous kinetic theory expressions can be derived for all of the transport coefficients. In particular, the thermal conductivity, the diffusion coefficients and the thermal diffusion coefficients are obtained by solving constrained singular linear systems. These approximate expressions are accurate and computationally much more cost-effective than a direct numerical inversion of the associated linear systems. Moreover, the approximate species diffusion coefficients and thermal diffusion coefficients automatically satisfy the mass conservation constraint (6).

Since radiation plays a key role in defining the structure and stability of flame-balls, it is necessary to construct a careful estimate of the radiation term q_R. We assume that for hydrogen-air mixtures the only significant radiating species is H_2O (For methane-air systems additional terms from CO and CO_2 will be included). By utilizing an optically thin limit in which self absorption of radiation is neglected, the divergence of the net radiative flux is given by

$$\frac{1}{r^2}\frac{d}{dr}(r^2 q_R) = 4\pi \sum_i \alpha_i B_i(T) \tag{7}$$

where $B_i(T)$ is the Planck function evaluated at the band centers of the contributing vibration-rotation or pure rotational bands whose integrated intensities are given by α_i [4,5].

To complete the specificiation of the problem, boundary conditions are needed at both ends of the computational domain. The boundary conditions in the fresh mixture are given by

$$T(\infty) = T_f, \quad Y_k(\infty) = Y_{k_f}, \quad k = 1, 2, \ldots, K. \tag{8}$$

Symmetry conditions at the origin are given by

$$\frac{dT}{dr}(0) = 0, \quad \frac{dY_k}{dr}(0) = 0, \quad k = 1, 2, \ldots, K. \tag{9}$$

Finally, we point out that the chemical production rates and transport coefficients are evaluated with optimized and highly efficient libraries [3,6].

Method of Solution

The equations in (1-4,7-9) form a nonlinear two-point boundary value problem. The solution method for a single solution has been discussed in detail elsewhere and we outline only the essential features here [7,8]. Our goal is to obtain a discrete solution of the governing equations on the finite difference mesh $\mathcal{M}$. By replacing the continuous differential operators by finite difference expressions, the problem of finding an analytic solution of the governing equations is converted into one of finding an approximation to this solution at each point of the mesh $\mathcal{M}$. We seek the solution U^* of the nonlinear system of difference equations

$$F(U) = 0. \tag{10}$$

Assuming we can obtain an initial solution estimate U^0 that is sufficiently "close" to U^*, the system of equations in (10) can be solved by Newton's method. We write

$$J(U^k)\left(U^{k+1} - U^k\right) = -\lambda_k F(U^k), \quad k = 0, 1, \ldots, \tag{11}$$

where U^k denotes the k^{th} solution iterate, λ_k the k^{th} damping parameter ($0 < \lambda \leq 1$) and $J(U^k) = \partial F(U^k)/\partial U$ the Jacobian matrix. A system of linear block tridiagonal equations must be solved at each iteration for corrections to the previous solution vector. As we found in the solution of burner-stabilized and freely propagating premixed laminar flames, the cost of forming (we use a numerical Jacobian) and factoring the Jacobian matrix can be a significant part of the cost of the total calculation. In such problems we apply a modified Newton method in which the Jacobian is re-evaluated periodically.

The solution of combustion problems, such as the flame-ball system, requires that the computational mesh be determined adaptively. We equidistribute the mesh $\mathcal{M}$ on the interval $[0, \infty]$ with respect to the non-negative function W and the constant C. Specifically, we form the mesh by employing a weight function that equidistributes the difference in the components of the discrete solution and its gradient between adjacent mesh points.

In addition to the generation of a single solution for these systems, we have studied the dependence of these flames (the flammability limits) on the equivalence ratio ϕ. While the solution method discussed above can be utilized to generate a single solution, it is not effective for the computation of solutions as one approaches turning points of the system. To be able to study flames in the neighborhood of extinction, we must apply a phase-space, pseudo-arclength continuation method with Newton-like iterations and global

adaptive gridding [9-11]. The set of governing equations for the flame-ball configuration reduces to a system of the form

$$\mathcal{F}(\mathcal{X}, \phi) = 0, \tag{12}$$

where $\mathcal{X} = (T, Y_1, \ldots, Y_K)$ is the solution vector. The solutions $(\mathcal{X}, \phi)$ in (12) form a one-dimensional manifold which, as a result of the presence of turning points, cannot be parameterized in the form $(\mathcal{X}(\phi), \phi)$. The upper part of the manifold denotes the stable solutions and the lower part the unstable ones assuming there are no Hopf bifurcations.

To generate this solution set, $(\mathcal{X}, \phi)$ is reparameterized into $(\mathcal{X}(s), \phi(s))$ where s is a new independent parameter and ϕ becomes an eigenvalue. The system in (12) can now be written

$$\mathcal{F}(\mathcal{X}(s), \phi(s)) = 0, \tag{13}$$

and the dependence of s on the augmented solution vector $(\mathcal{X}, \phi)$ is specified by an extra scalar equation

$$\mathcal{N}(\mathcal{X}(s), \phi(s), s) = 0, \tag{14}$$

which is chosen such that s approximates the arclength of the solution branch in a given phase space. Rather than solving the coupled system in (13) and (14), we replace ϕ by a function ϕ of z and we let the unknown $\mathcal{Z} = (\mathcal{X}^T, \phi)^T$ be the solution of a three-point limit value problem

$$\mathcal{H}(\mathcal{Z}, s) = \begin{bmatrix} \mathcal{F}(\mathcal{X}, \phi) \\ \dfrac{d\phi}{dz} \\ \mathcal{N}(\mathcal{X}(\hat{z}), \phi(\hat{z}), s) \end{bmatrix} = 0, \tag{15}$$

where $\hat{z}$ is a given point in $[0, \infty]$. The system in (15) is solved by combining a first-order Euler predictor and a corrector step involving Newton-like iterations and adaptive gridding.

Numerical Results

During the first eight months of the project our goals have included verifying the sensitivity of the flame ball radius and the value of the lean and rich flammability limits to 1) the hydrogen-air chemistry, 2) the transport model and 3) the radiation approximation. Our previous hydrogen-air flame ball computations [12] employed a Curtiss-Hirschfelder transport approximation with a radiation model in which interpolated emissivity data was used to construct an approximation for the divergence of the radiative heat flux.

Utilizing a modified hydrogen-air reaction mechanism [13] with the transport model employed in [12], we computed flame balls as a function of the equivalence ratio ϕ. Temperature and radii results are compared with our original computations in Figures 1a and 1c. While the temperature and the size of the flame ball at the rich limit show only minor changes, there is a modest increase of the rich flammability limit with the new mechanism. Only very small changes occur on the lean side but they move in the direction of increased agreement with the experiments [12]. In Figures 1b and 1d we compare the temperature and radii as a function of the equivalence ratio for the new mechanism/old transport calculations with calculations made with the new mechanism and the transport and radiation models discussed above. Essentially no major differences were found. Nevertheless, due to its more accurate formulation, the detailed transport and band radiation models will be utilized in all future flame ball calculations.

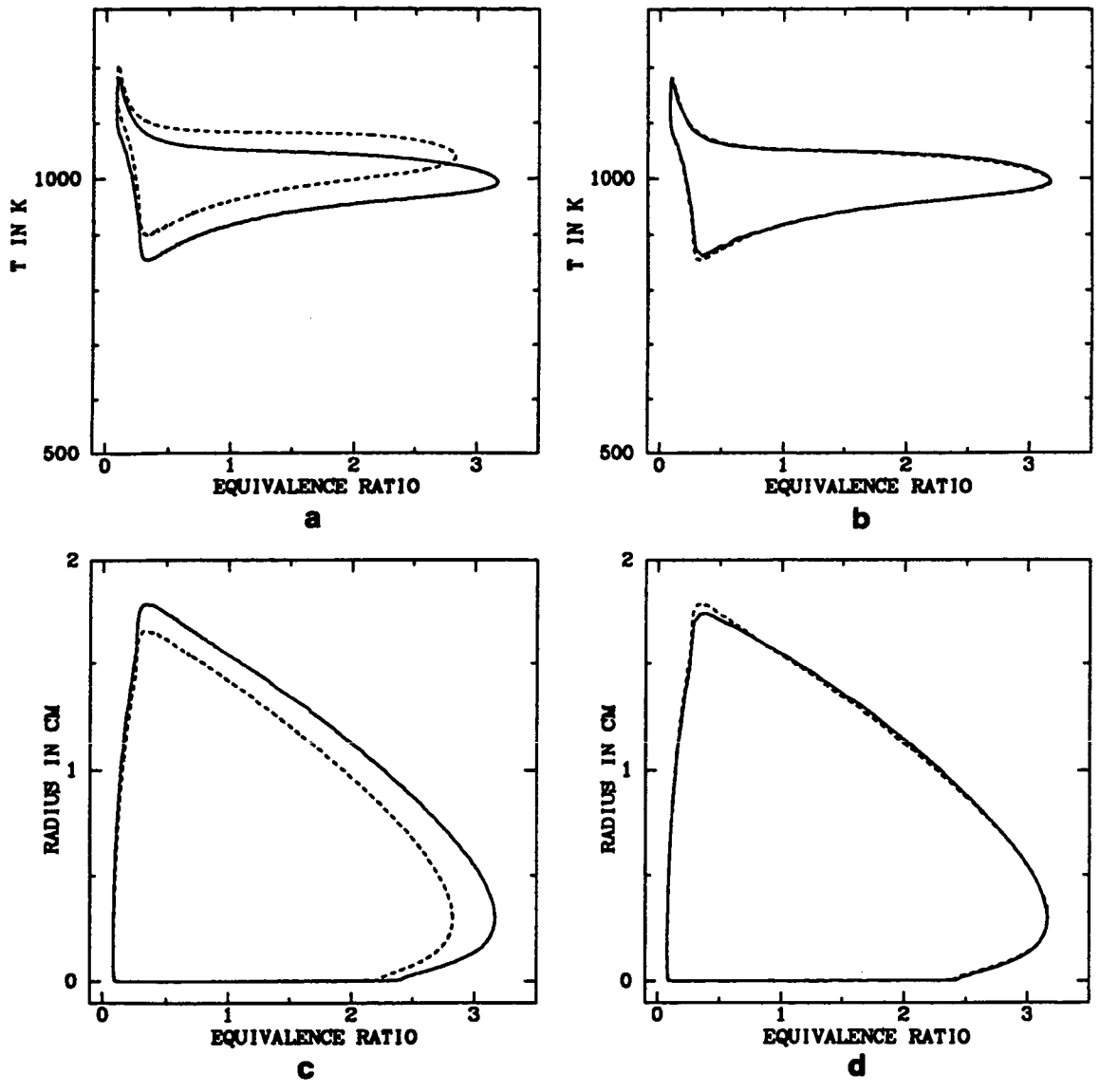

Figure 1 (**a**) A comparison of the temperature versus the equivalence ratio for hydrogen-air flame balls utilizing the old mechanism and old transport (dash) with computations utilizing the new mechanism and old transport (solid); (**b**) a comparison of the temperature versus the equivalence ratio for the new mechanism and old transport (dash) with computations utilizing the new mechanism, transport and radiation models (solid); (**c**) a comparison of the flame ball radius versus the equivalence ratio for the old mechanism and old transport (dash) with computations utilizing the new mechanism and old transport (solid); (**d**) a comparison of the flame ball radius versus the equivalence ratio for the new mechanism and old transport (dash) with computations utilizing the new mechanism transport and radiation models (solid).

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