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Rarefied flow effects on stabilization and extinction of rotating-disk flame at low pressures

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ABSTRACT

An activation energy asymptotic analysis with one-step overall reaction was performed for the stabilization and extinction of a premixed flame over a rotating disk at sufficiently low pressures, for its relevance in low-pressure CVD (chemical vapor deposition) operations in which the flow is weakly rarefied. Extinction criteria based on the critical Damköhler number were obtained through the S-curve concept, parametrically demonstrating the influence of the CVD operating conditions, such as the spin rate and temperature of the disk, on flame extinction. It is further shown that, while decreasing pressure and hence the reactivity of the mixture tends to extinguish the flame, the trend can be substantially weakened by taking into account of the influence of the Knudsen layer, which reduces the heat loss to the disk as well as the flow stretch rate at the flame.

1. Introduction

Flame-assisted chemical vapor deposition (FACVD) has been widely used for diamond film synthesis [1–7]. In such a reactor, a premixed flame is stabilized over a heated substrate impinged by a fuel-rich ethylene–oxygen mixture flow, such that the reaction products from the flame are brought toward and subsequently deposited on the substrate through surface reactions. In order to obtain desirable properties of the film, studies have been conducted to identify optimum operating conditions of FACVD, such as the fuel type, the equivalence ratio, the substrate temperature, the flow type and the system pressure. For example, it was experimentally observed that large area coverage and high uniformity of the diamond deposition can be achieved by reducing the system pressure [1–7] and/or spinning the substrate to stretch the flame [5]. Since operation of FACVD requires a steady flame, which however could be extinguished by increasing the spin rate of the rotating substrate and/or decreasing the system pressure, an analysis yielding the parametric influence of the operating conditions on the state of flame extinction is of practical interest.

The problem of interest involves an infinite disk rotating about its symmetry axis in a stationary fluid composed of a chemically reacting mixture. The fluid near the disk surface is thrown outward through spinning and a compensating flow is accordingly induced to impinge the disk. Due to the self-similar nature of the rotating-disk flow [8,9], the axial velocity, temperature and species concentration only depend on the axial distance from the disk, and a flat flame can be stabilized over the disk for appropriate operating conditions. Consequently, such a flow configuration has the advantage of synthesizing films with high uniformity and large area coverage. It is noted that, while the self-similar character of the rotating-disk flow exists only for a disk with infinite radius, it is nevertheless a good approximation for a finite disk, over a large fraction of the radial direction, when the spin rate is sufficiently large [10,11].

It has also been experimentally demonstrated, say for diamond deposition, that the film uniformity and coverage can be promoted by operating the FACVD at low pressures. The enhancements arise from the suppression of unwanted gas-phase reactions and thereby the improved purity of the film, and the controllability of the substrate temperature. However, in the prevalent pressure range, rarefied gas effects could be important and as such need to be considered in the analysis. Mechanistically, we recognize that the rotating-disk flow has a boundary-layer-like flow structure, whose characteristic length is about 1.0 mm in atmospheric pressure for characteristic spin rates of 800–1000 rpm, and is inversely proportional to the square root of the pressure, while the mean free path of the gas mixture is about 10^{-4} mm in one atmosphere and is inversely proportional to the pressure. As a consequence of decreasing the pressure, the Knudsen number, *Kn*, which is a measure of the gas rarefaction and is defined as the ratio of the mean free path to the characteristic length, could increase to $O(10^{-3}–10^{-1})$ in the operating conditions of FACVD, and as such renders the flow to be weakly rarefied.

Physically, the weakly rarefied rotating-disk flow consists of a continuum boundary-layer flow with the Knudsen layer next to the disk, in which the distribution function of gas molecules is generally non-Maxwellian, and the continuum description is not valid.

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To account for effects of the Knudsen layer, weakly rarefied flows are conventionally studied in the framework of the continuum mechanics but with appropriate slip boundary conditions [12,13], indicating the concept that the physical properties (e.g. velocity, temperature and concentration) of the flow at the disk, as perceived by the flow, are not the same as those of the disk but instead possess a certain amount of slip. It is expected that the presence of slip properties will change the velocity, temperature and concentration profiles of the rotating-disk flow field and hence influence the flame extinction.

Asymptotic analysis of flame extinction based on the large activation energy assumption of a one-step overall reaction is well established in combustion theory, and has been performed for various situations involving stagnation and boundary-layer flows [14–16]. The present analysis can therefore be considered as an extension of the existing theories to rotating-disk flows, yielding information on the extinction characteristics of a reactive system through the S-curve analysis, which describes the response of the flame intensity to the system Damköler number, *Da*, defined as the ratio of the characteristic flow time to the characteristic reaction time. A steady flame cannot be sustained when *Da* becomes smaller than a critical value – the extinction Damköler number, which is identified as the turning point of the upper-half of the S-curve. Thus, the primary objective of the present study is to obtain the S-curve of the rotating-disk flame, identify the corresponding extinction Damköler number, and elucidate their dependence on the flow conditions, especially on the pressure. Formulation of the present problem will be presented in the next section, followed by the extinction analysis and results in Section 3.

2. Formulation

2.1. Governing equations

We consider a steady axisymmetric rotating-disk flow for a chemically reacting mixture with variable properties. A cylindrical coordinate system (r, ϕ, z) is so established that the disk is located on the plane $z = 0$ and rotates about the z-axis with an angular velocity Ω; the flow velocity components are denoted by (u, v, w) corresponding to (r, ϕ, z), respectively. The governing equations for the flow are given by the continuity equation,

$$\frac{1}{r}\frac{\partial}{\partial r}(r\rho u) + \frac{\partial}{\partial z}(\rho w) = 0, \tag{1}$$

the radial momentum equation,

$$\rho\left(u\frac{\partial u}{\partial r} + w\frac{\partial u}{\partial z} - \frac{v^2}{r}\right) = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial r}\left\{2\mu\frac{\partial u}{\partial r} - \frac{2}{3}\mu\left[\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{\partial w}{\partial z}\right]\right\} + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right)\right] + \frac{2u}{r}\left(\frac{\partial u}{\partial r} - \frac{u}{r}\right), \tag{2}$$

the circumferential momentum equation,

$$\rho\left(u\frac{\partial v}{\partial r} + w\frac{\partial v}{\partial z} + \frac{uv}{r}\right) = \frac{\partial}{\partial r}\left[\mu\left(\frac{\partial v}{\partial r} - \frac{v}{r}\right)\right] + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v}{\partial z}\right)\right] + \frac{2u}{r}\left(\frac{\partial v}{\partial r} - \frac{v}{r}\right), \tag{3}$$

the axial momentum equation,

$$\rho\left(u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial z}\right) = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial z}\left\{2\mu\frac{\partial w}{\partial z} - \frac{2}{3}\mu\left[\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{\partial w}{\partial z}\right]\right\} + \frac{1}{r}\frac{\partial}{\partial r}\left[\mu r\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right)\right], \tag{4}$$

the species equation,

$$\rho\left(u\frac{\partial Y}{\partial r} + w\frac{\partial Y}{\partial z}\right) - \left[\frac{\partial}{\partial r}\left(\rho D\frac{\partial Y}{\partial r}\right) + \rho D\frac{1}{r}\frac{\partial Y}{\partial r} + \frac{\partial}{\partial z}\left(\rho D\frac{\partial Y}{\partial z}\right)\right] = -\omega, \tag{5}$$

the energy equation,

$$\rho c_p\left(u\frac{\partial T}{\partial r} + w\frac{\partial T}{\partial z}\right) - \left[\frac{\partial}{\partial r}\left(\lambda\frac{\partial T}{\partial r}\right) + \lambda\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)\right] = q_c\omega, \tag{6}$$

and the ideal gas law,

$$p = \rho R^o T/\overline{W}, \tag{7}$$

where ρ is the density, p the pressure, T the temperature, μ the viscosity, D the mass diffusivity, λ the thermal diffusivity and R^o the universal gas constant. The average molecular weight of the mixture $\overline{W}$, the specific heat capacity c_p and the heat of combustion q_c are assumed to be constants. In deriving (5) and (6), we have assumed that the mixture is sufficiently off-stoichiometric that the reaction is governed by the mass fraction Y of the deficient reactant, which corresponds to the oxidizer in the fuel-rich hydrocarbon–oxygen mixture, and hence a one-reactant, one-step overall reaction, Reactant → Products, is used in the present formulation. This assumption is consistent with the fact that very rich ethylene–oxygen flames are employed in FACVD for the deposition of diamond films. Consequently, the reaction rate ω can be expressed by $\omega = B\rho^n Y e^{-E_a/R^oT}$, where the overall reaction order n is close to 2 at low pressures; the activation energy E_a and the collision rate factor B can be treated as constants [16]. It is noted that we have neglected the expansion work by the pressure and the viscous dissipation in (6) since they are negligibly small compared to the chemical heat release.

Eqs. (1)–(7) are to be solved subject to the boundary conditions at infinity,

$$u = v = 0, \quad T = T_\infty, \quad Y = Y_\infty, \tag{8}$$

where the subscript ∞ denotes the physical quantities at $z = \infty$, and the slip boundary conditions at the disk [13,17,18],

$$u = \frac{2-\alpha_V}{\alpha_V}l_m\frac{\partial u}{\partial z}, \quad v = \Omega r + \frac{2-\alpha_V}{\alpha_V}l_m\frac{\partial v}{\partial z}, \quad w = 0, \tag{9}$$

$$T = T_w + \frac{2-\alpha_T}{\alpha_T}\frac{2\gamma}{1+\gamma}\frac{1}{Pr}l_m\frac{\partial T}{\partial z}, \quad \frac{\partial Y}{\partial z} = 0, \tag{10}$$

where l_m is the mean free path of gas molecules, α_V the accommodation coefficient for velocity, α_T the accommodation coefficient for temperature, γ the heat capacity ratio and Pr the Prandtl number. In deriving (9) and (10), we have neglected the chemical deposition of gas species at the disk since the deposition rate is usually so small that the induced axial velocity at the disk surface and the concomitant heat release have negligible influence on the flow.

2.2. Similarity formulation

Following the approach of von Kármám [8] and Ostrach and Thornton [19], we seek a similarity solution of (1)–(7) in the form

$$u(r,z) = \Omega r F(\zeta), \quad v(r,z) = \Omega r G(\zeta), \quad w(r,z) = (\rho_\infty/\rho)\sqrt{\Omega v_\infty}H(\zeta), \tag{11}$$

$$T(r,z) = (Y_\infty q_c/c_p)\widetilde{T}(\zeta), \quad Y(r,z) = Y_\infty\widetilde{Y}(\zeta), \quad p(r,z) = \rho_\infty v_\infty \Omega P(z), \tag{12}$$

where $\zeta = \sqrt{\Omega/v_\infty}\int_0^z \rho(\eta)/\rho_\infty d\eta$ is a non-dimensional coordinate and $v = \mu/\rho$ the kinematic viscosity. Noting that the pressure vari-