Numerical study of the influence of gas expansion on the acceleration of outwardly expanding flames

Ruixue Feng^{1,3}, Ruiming Zhang^{1,3}, Damir Valiev^{1,2,3}

¹Center for Combustion Energy, Tsinghua University, Beijing 100084, China
²Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Tsinghua University, Beijing 100084, China
³Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China

Abstract

The role of Darrieus-Landau instability in wrinkling the initially smooth freely propagating expanding flame front has been studied by solving the two-dimensional Navier–Stokes equations with one step irreversible Arrhenius reaction. Numerical simulation of the radially expanding flames indicates a power law temporal dependence of mean radius after a certain critical time instant. Influence of gas expansion ratio on power-law exponent and flame surface dimension is the focus of this research. It is shown that the expansion coefficient has a considerable effect on fractalization behavior of the flame, confirming the assumption that fractal dimension is not a universal parameter.

1 Introduction

The flame front of freely propagating premixed flame in a gaseous combustible mixture can be affected by hydrodynamic instability, which is known as Darrieus-Landau (DL) instability. DL instability appears differently in flame in tubes and in freely expanding flames. Development of the DL instability wrinkles the smooth flame front and, as a result, the surface area and velocity of a flame increase. A spherical flame, as it propagates outward, develops a multiple-scale surface resembling a fractal. Small scale humps grow, and when their size exceeds a certain value, smaller humps start to grow on their surface, and this cascading of hump growth leads to fractalization of the flame surface [1]. The growth of flame front is a process controlled by the overall expansion. Basic idea of flame fractalization can be understood using Koch curve [2]. It has been found that wrinkled flame accelerates, which can be approximated as $R \propto At^{\alpha}$; $U_W = dR/dt \propto At^{(\alpha-1)}$, where R(t) is the average radius of the wrinkled flame ball, A is an empirical constant, and α is a non-dimensional power exponent [1]. For a Koch curve, the size of triangles decreases

by a factor *b* at every cascade step: $L_{k+1} = L_k / b$. At the same time, total length of the curve increases by a factor β , $S_{k+1} = \beta S_k$. For 2-D geometry, the fractal dimension is 1+d, where *d* is the fractal excess, $d = (\alpha - 1) / \alpha$ [3,7]. In the case of 3-D geometry, fractal dimension is 2+d. The cascade process is limited by the smallest and largest triangle scale λ_{\min} and λ_{\max} ; for a very large number of steps N >> 1, we have $\lambda_{\max} = \lambda_{\min} b^N$ [3].

For freely propagating spherical flames, experimental data shows [1] that the value of the fractal dimension is consistent with the self-similar behavior with $\alpha = 3/2$, implying d = 1/3 and fractal dimension 1.33 accordingly. The radial growth with 3/2 power law was observed for 2-D cases [4,5,6], which contradicted the dimension of the problem [3]. Resolving the contradiction between power law exponents in 2D and 3D geometries needed additional studies [7,8,9].

Some numerical results [5,10] are obtained using the scaled form of equations which are independent of the expansion ratio, indicating that the fractal dimension obtained through this statement may only be a constant. However, Blinnikov and Sasorov [11] suggested that larger expansion coefficient leads to a more wrinkled flame front. In Ref. [12], a method for estimating the acceleration exponent from the global pulsations of the flame front that are induced by wrinkling has been proposed. Recent experiments [13] showed that the acceleration exponent weakly depends on equivalence ratio, with both Darrieus-Landau and diffusional-thermal instabilities wrinkling the flame front. In Ref. [14], it has been shown experimentally that the acceleration exponent weakly depends on expansion for a relatively narrow range of expansion ratios. The above results indicate that it is essential to further investigate whether the fractal flame dimension depends on the gas expansion ratio. We perform a detailed investigation of the role of gas expansion on the acceleration and fractal properties of freely outwardly propagating flame for Le=1 and a wider range of expansion ratio and acceleration exponent.

2 Numerical simulation

Numerical simulation is set to solve Navier-Stokes equations for unsteady compressible reacting flow with one-step irreversible chemical Arrhenius reaction. The governing equations are as follows [7]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + \delta_{ij} P - \tau_{ij}) = 0$$

$$\frac{\partial}{\partial t} (\rho e_0 + \frac{1}{2} \rho u_j u_j) + \frac{\partial}{\partial x_i} (\rho h_0 u_i + \frac{1}{2} \rho u_i u_j u_j - q_i - u_j \tau_{ij}) = 0$$

$$\frac{\partial}{\partial t} (\rho Y) + \frac{\partial}{\partial x_i} (\rho Y u_i - \frac{\mu}{\text{Sc}} \frac{\partial Y}{\partial x_i}) = -\frac{\rho Y}{\tau_R} \exp(-E / RT)$$
(1)

where Y is the fuel mass fraction, $e = QV + C_V T$ is the internal energy, $h = QV + C_P T$ is the enthalpy, Q is the energy release. C_V and C_P are the specific heat capacity at constant volume and pressure respectively. The stress tensor and the energy diffusion vector are given by

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$$\tau_{ij} = \mu \frac{\partial u_i}{\partial x_j} + \mu \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k}$$
(2)

$$q_{i} = C_{p} \frac{\mu}{\Pr} \frac{\partial T}{\partial x_{i}} + Q \frac{\mu}{\operatorname{Sc}} \frac{\partial Y}{\partial x_{i}}$$
(3)

where μ is the fuel viscosity coefficient, Pr is the Prandtl number, and Sc is Schmidt number. Here we take Pr = Sc = 0.5, considering the negligible effect of viscosity during the flame evolution, and take Le = Pr/Sc = 1, avoiding thermal-diffusion instability. We assume that the gas is a perfect mixture satisfying the law of ideal gas:

$$P = \frac{R}{m}\rho T \tag{4}$$

where *R* is the universal gas constant and *m* is molecular weight which equals to 0.029 kg/mol. The reaction rate is given by the Arrhenius law with the activation energy *E* and a constant with the dimension of time, τ_R . The factor τ_R was adjusted to obtain a particular value of the planar laminar flame velocity S_L by solving the associated eigen-value problem.

The thermal and chemical parameters of the model fuel mixture were chosen to reproduce the most important properties of typical laboratory flames [15]. The initial conditions are: temperature T = 300 K, pressure $P = 10^5$ Pa , density $\rho_0 = 1.16$ kg/m³ , dynamic viscosity coefficient $\mu = 1.7 \times 10^{-3}$ Ns/m² , specific heat $C_p = 7R/2m$. Thermal expansion ratio, one of the key parameters for the parametric study, is taken in the range $\Theta \equiv \rho_0 / \rho_b = 5 - 14$, where ρ_b is the burnt gas density. The energy release is given as $Q = C_p T_f (\Theta - 1)$. We employed a scaled activation energy $E / \theta R T_f = 4$. We define flame Mach number $Ma = S_L / c_u = 0.005$, where c_u is the sound speed at the reactants. The flame thickness is conventionally defined as [16]:

$$\delta_L = \frac{\mu}{\Pr \rho_0 S_L} \tag{5}$$

The solver is based on a cell-centered, finite-volume numerical scheme, for 2-D unsteady compressible viscous Navier-Stokes equations. The flame front is initialized using Zeldovich-Frank-Kamenetskii -like flame structure [7,15].

In present study, a nonuniform Eulerian calculation grid shaped as a 90° annular sector is used. The mesh in the subdomain near the flame front is uniform and adaptive, which is rearranged automatically during the calculation to capture the propagating flame dynamically. The cell size of adaptive mesh in a flame subdomain is constant $(0.5\delta_L)$. It is noted that δ_L is defined from dimensional considerations, with thermal flame thickness being several times larger. For that reason, the chosen spatial resolution is adequate, which is supported by resolution tests. For the inner and outer zone of an annular core, we set the mesh nonuniform of which the grid size will be increased by a certain rate. Splines of the third order are used for reinterpolation of the flow variables during periodic grid reconstruction to preserve the second order accuracy of the numerical scheme. DL instability is triggered by a perturbation in the form of infinitesimal numerical noise. Grid independence tests for freely propagating curved flame show the convergence of curved flame speed with increasing spatial resolution.



Figure 1. (left) Flame front evolution for Θ =8; (right) Mean flame radius vs time (log-log) for Θ =5, 8, 12, 14.

3 Results and discussion

Simulations are performed over a wide range of expansion ratio Θ =5, 8, 12, 14. We set a circular initial flame front with the radius $R = 100\delta_t$ at the computational grid.

Fig. 1 (left) presents a flame front illustrated by the temperature isotherms for Θ =8, at equally spaced time instants (with Δ t=0.03 s) from the beginning (t=0 s) to the stage of fully developed fractal-like structure, (t=0.24 s). With the flame propagating and DL instability developing, the initial smooth flame front start to wrinkle and form the cusps, leading to an expansion of surface area and the increase of flame velocity. During the flame propagation, humps grow in amplitude, and their size eventually will be limited by the largest length scale $2\pi R / n_c$, where n_c is the critical spherical harmonic number. Any perturbation larger than this value can't develop, since the front curvature is finite. The smallest size is limited by cut-off wavelength $\lambda_c \approx 20\delta_L$, according to theoretical estimate [3]. As the scale of cusps grow, smaller humps begin to develop on the previous ones, which leads to hierarchy of hump formation during the flame evolution. The same phenomena will appear when the small humps get into larger ones, consequently, form a fractal structure.

Fig. 1 (right) presents a log-log plot of flame radius evolution for Θ =5, 8, 12, 14. The dashed lines with fixed slopes show the approximation of R(t) dependence at self-similar propagation stage with a power law. The plots show a clearly visible power law relationship between the mean flame radius and time at a later stage. After the initial transient time, a constant slope of R(t) dependence in log-log plot is observed, consistent with $R \propto At^{\alpha}$. At the transient point, the flame front starts to attain a fractal-like structure and propagate in a self-similar regime. As summarized in Table 1, for different expansion ratios, α attains different values: the larger is the expansion ratio, the faster the acceleration and the steeper is the slope. Next, we compare numerically obtained values of α to theoretical estimates.

In 2-D geometry, the theoretically predicted factor β (total length increasing rate) depends on expansion ratio as [3]

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$$\beta_{2D} = 1 + \Theta / 2[(\Theta - 1)^2 / (\Theta^3 + \Theta^2 + 3\Theta - 1)]$$
(6)

The factor *b* (increase of the length scale for a fractal generator) is given as $b = R_W / R_C$, where R_w is the critical tube width below which all perturbations of the curved flame are damped, R_c is the second critical value of the tube width corresponding to a stability limit of a curved flame. The theoretical estimate within the stability limits of a curved laminar flame gives the value $R_W / R_C = 4 - 5$ [17] for expansion ratios in the range $\Theta = 5 - 10$, $R_W / R_C = 4$ for $\Theta = 5$, and $R_W / R_C = 5$ for $\Theta = 10$, respectively. The fractal excess *d* is given by $d = \ln \beta / \ln b$, while the power of radial growth given by $\alpha = 1/(1-d)$. Thus, we are able to calculate β and *d* in the terms of different expansion ratio, as shown in Table 1. Here, α_{theor} is the power exponent calculated according to the theory, α_{num} is the power exponent obtained through the fitting of the data from numerical simulation.

It is noted that the range of expansion ratios Θ used in Ref. [17] to estimate *b* doesn't cover the whole range of Θ that we choose for present simulations, which results in a need to extrapolate values of *d* for larger expansion ratios. A more accurate estimate of *d* requires a separate large-scale parametric study for freely propagating flames and will be presented elsewhere.

	β_{2D}	b	d _{2D}	α_{theor}	α_{num}
Θ=5	1.244	4	0.157	1.186	1.119
Θ=8	1.327	4.6	0.185	1.227	1.154
Θ=12	1.381	5.4	0.201	1.252	1.241
Θ=14	1.397	5.8	0.207	1.261	1.284

Table 1: Fractal parameters different expansion ratios.

4 Conclusions

Comparing theoretical and simulation results, we can draw the following conclusions. As mentioned earlier, the power exponent in R(t) dependence is often considered a constant without taking the gas expansion into account. However, theoretical estimate of α is dependent on fractal dimension [1], which is affected by β and *b*. Both β and *b* turn out to have a dependence on expansion ratio. As a result, according to theory [3], α is expected to vary over the range of expansion ratios, growing with the increase of Θ . The theoretical estimate of α is consistent with what we obtain from the numerical simulations. After a certain transitional period, R(t) has a power-law dependence on time t, $R \propto At^{\alpha}$. For different expansion ratio, α is growing with increasing expansion ratio.

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