

Initiation and evolution of triple flames subject to thermal expansion and gravity

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Abstract

We investigate the combined effects of thermal expansion and gravity on the initiation and evolution of triple flames. In particular, we provide a possible criterion for the thermal energy per unit depth required for triple flame ignition by a cylindrical ignition kernel. Further, we describe the transient evolution of triple flames after initiation. Steady, non-propagating, planar solutions representing “flame tubes” are determined. The flame tube solutions are unstable; in time-dependent simulations it is found that initial perturbations increasing the thermal energy of flame tubes lead to the propagation of a triple flame, while perturbations decreasing the thermal energy lead to extinction. Therefore it is concluded that the thermal energy of flame tubes may be used to define a possible ignition energy per unit depth for planar triple flames in the mixing layer, analogous to spherical flame balls for spherically expanding flames. This is the first paper to provide a detailed study of the ignition energy of planar triple flames. When gravity is not taken into account, flame tubes subject to thermal expansion are found not to induce a flow, so that the flame tube energy can be determined without having to solve the full Navier–Stokes equations.

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Keywords: Flame dynamics; Triple flames; Ignition; Buoyancy effects; Flame tubes

1. Introduction

Understanding the transient dynamics of a flame from initiation to steady propagation, and in some cases instability, is a vital part of fundamental combustion research. In this paper we study the problem of triple flame initiation in a mix-

ing layer, taking the combined effects of thermal expansion and gravity into account. In particular, we provide a possible criterion for the ignition energy per unit depth of a triple flame from a cylindrical ignition kernel generated, for example, by a hot wire. Further, we study the transient evolution of triple flames after initiation.

The problem of ignition in homogeneous mixtures, which leads to the propagation of premixed flames, has been the focus of a large amount of research. In the particular case of spherically expanding premixed flames, a possible theoretical cri-

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terion for the energy required for ignition is provided by the thermal energy in the burnt gas of a non-propagating, spherically symmetric solution of the governing equations known as a Zeldovich flame ball [1]. Flame balls have been found to be typically unstable under adiabatic conditions, and small perturbations can lead to either an outwardly propagating flame or an inwardly propagating flame and eventual extinction [1–4]. Further studies in the literature have investigated the transient dynamics of spherical premixed flames from an initial ignition kernel, depending on aspects such as heat loss and Lewis numbers (see e.g. [5–8]).

There has been considerably less focus on flame ignition in situations where the reactants are non-premixed. The work that has been done on both laminar and turbulent non-premixed ignition is summarised in the detailed review paper [9]. Most studies on non-premixed flame ignition have been concerned with autoignition, sometimes referred to as “self-ignition”. There are very few papers that have investigated the energy required for “forced ignition” of non-premixed flames by an external heat source or spark. The transient dynamics of flames in inhomogeneous mixtures from forced ignition has been investigated using Direct Numerical Simulations (DNS) in the laminar case in [10,11], and more recently with the effects of turbulence included in [12–15]. These numerical studies do not, however, contain a detailed investigation of the energy required for ignition. To our knowledge there have been no dedicated investigations of the energy required for forced ignition of laminar planar triple flames in mixing layers.

Some recent papers have extended the concept of Zeldovich flame balls to the inhomogeneous case, describing theoretically [16] and numerically [17] the existence and properties of flame balls in reactive mixing layers. Similarly to Zeldovich flame balls, these inhomogeneous flame balls may provide a corresponding criterion for the minimum energy for the successful ignition of axisymmetric flames in the mixing layer. Here we extend the current understanding of flame ignition by providing a criterion for the minimum ignition energy for triple flames in the mixing layer, via a cylindrical ignition kernel. This is achieved by first investigating steady, planar, non-propagating solutions of the governing equations which we refer to as “flame tube” solutions. Such solutions have been observed in previous numerical simulations [18–21] where the planar solutions are prone to cellular instabilities due to Lewis number effects [19], but these studies were not concerned with ignition. More relevant to the ignition problem are the papers [22] and [23]. These studies include investigations of “flame isolas” and “flame disks”, respectively, which are axisymmetric, stationary solutions of the governing equations. Although [22] and [23] only partially address the ignition problem, in the paper [23], non-propagating

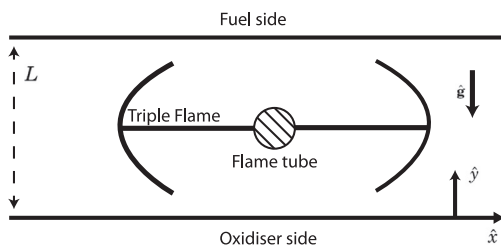


Fig. 1. An illustration of a pair of triple flames in a planar channel of height L . Also illustrated on the diagram is the stationary, non-propagating “flame tube” solution that is used as initial condition in the transient triple flame simulations throughout the paper.

“flame disk” solutions are argued to indicate that a minimum energy is required for ignition of axisymmetric flames in the mixing layer. To our understanding, no such study has yet been performed for planar triple flames in the mixing layer, as investigated in this paper.

In this paper, we also investigate the transient evolution of propagating triple flames. Steadily propagating triple flames are well studied. Aspects of these structures that have been investigated include preferential diffusion [24,25], heat losses [26–28], reversibility of the chemical reaction [29,30], the presence of a parallel flow [31] and thermal expansion [32,33]; for further references see the review papers [20] and [34]. Here we are specifically interested in the combined effects of thermal expansion and gravity on the transient dynamics of triple flames, in situations where the planar diffusion flame is stable [35].

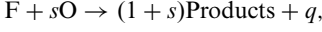
The paper is structured as follows. In Section 2 we formulate the problem and describe the numerical procedure. In Section 3 we provide the results obtained from the numerical solution of the governing equations. We end the paper with conclusions and recommendations for future work in Section 4.

2. Formulation

We investigate triple flame propagation in an infinitely long channel of height L , where fuel is provided at the upper wall and oxidiser at the lower wall (Fig. 1). The walls are taken to be rigid, porous, isothermal and of equal temperature. This configuration has been used in several previous studies, by ourselves and others (e.g. [22,31,33,35,36]). We believe this configuration is difficult, but not necessarily impossible, to achieve experimentally. From previous investigations, we expect the results obtained in the current configuration to hold, at least qualitatively, in the 2D counterflow configuration.

The governing equations for temperature, fuel and oxidiser are coupled to the Navier–Stokes

equations for the fluid velocity vector $\hat{\mathbf{u}}$ to take thermal expansion and gravity $\hat{\mathbf{g}}$ into account. For simplicity, the combustion is modelled as a single, irreversible, one-step reaction of the form



where F denotes the fuel and O the oxidiser; s denotes the mass of oxidiser consumed and q the heat released, both per unit mass of fuel. The overall reaction rate $\hat{\omega}$ is taken to follow an Arrhenius law of the form

$$\hat{\omega} = \hat{\rho} B \hat{Y}_F \hat{Y}_O \exp(-E/R\hat{T}).$$

Here $\hat{\rho}$, \hat{Y}_F , \hat{Y}_O , R , \hat{T} , B and E are the density, the fuel mass fraction, the oxidiser mass fraction, the universal gas constant, the temperature, the pre-exponential factor and the activation energy of the reaction, respectively.

2.1. Governing equations and boundary conditions

We adopt the low Mach number formulation and assume that $\hat{\rho}D_T$, $\hat{\rho}D_F$ and $\hat{\rho}D_O$ are constant, where D_T , D_F and D_O are the diffusion coefficients of heat, fuel and oxidiser, respectively. We also assume that the specific heat capacity c_p , the thermal conductivity λ and the dynamic viscosity μ are constant.

In this paper, we are concerned with the initiation of a pair of triple flames, which are expected to propagate in opposite directions [10,11]; we therefore impose symmetry conditions at the centreline, which we take to be located at $\hat{x} = 0$, and solve the problem for $\hat{x} \geq 0$. In the unburnt gas at $\hat{x} = \pm\infty$ we assume that the induced flow is fully developed and the temperature and mass fractions are “frozen”, denoted with a subscript u . The walls are assumed to be rigid and to have equal temperatures $\hat{T} = \hat{T}_u$. The mass fractions are prescribed by $\hat{Y}_F = \hat{Y}_{Fu}$, $\hat{Y}_O = 0$ at the upper wall and $\hat{Y}_F = 0$, $\hat{Y}_O = \hat{Y}_{Ou}$ at the lower wall.

Non-dimensional variables are defined by

$$\left. \begin{aligned} x &= \frac{\hat{x}}{L}, y = \frac{\hat{y}}{L}, u = \frac{\hat{u}}{S_L^0}, v = \frac{\hat{v}}{S_L^0}, \\ t &= \frac{\hat{t}}{L/S_L^0}, \theta = \frac{\hat{T} - \hat{T}_u}{\hat{T}_{ad} - \hat{T}_u}, y_F = \frac{\hat{Y}_F}{\hat{Y}_{F,st}}, \\ y_O &= \frac{\hat{Y}_O}{\hat{Y}_{O,st}}, p = \frac{\hat{p}}{\hat{\rho}_0(S_L^0)^2}. \end{aligned} \right\} \quad (1)$$

The subscript “st” denotes values at the stoichiometric surface located at $\hat{y} = Y_{st}$, where in the unburnt gas

$$\frac{Y_{st}}{L} = \frac{1}{1 + S}. \quad (2)$$

Here $S \equiv s\hat{Y}_{Fu}/\hat{Y}_{Ou}$ is a normalised stoichiometric coefficient. The quantity $\hat{T}_{ad} \equiv \hat{T}_u + q\hat{Y}_{F,st}/c_p$ is the adiabatic flame temperature and S_L^0 is the laminar burning speed of the stoichiometric planar flame to

leading order for $\beta \gg 1$,

$$S_L^0 = \left(\frac{4Le_F Le_O}{\beta^3} Y_{O,st} (1 - \alpha) D_T B \exp(-E/R\hat{T}_{ad}) \right)^{1/2},$$

where $Le_F = D_T/D_F$ and $Le_O = D_T/D_O$ are the fuel and oxidiser Lewis numbers, respectively, $\beta \equiv E(\hat{T}_{ad} - \hat{T}_u)/R\hat{T}_{ad}^2$ is the Zeldovich number or non-dimensional activation energy and $\alpha \equiv (\hat{\rho}_u - \hat{\rho}_{ad})/\hat{\rho}_u$ is the thermal expansion coefficient. We set the Lewis numbers equal to unity in order to concentrate on the effects of thermal expansion and gravity on triple flames, without the complication of thermo-diffusive instabilities. Following the method of [35], we note that for unity Lewis numbers the *mixture fraction* Z , defined as

$$Z = \frac{y_F + \theta}{1 + S} = 1 - \frac{S}{1 + S}(y_O + \theta) \quad (3)$$

satisfies the reaction-free equation

$$\rho \frac{\partial Z}{\partial t} + \rho \mathbf{u} \cdot \nabla Z = \epsilon \nabla^2 Z. \quad (4)$$

We can therefore solve Eq. (4) and use Eq. (3) to find the fuel and oxidiser mass fractions if required. Thus the non-dimensional governing equations can be written

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0, \quad (5)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \epsilon Pr \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla(\nabla \cdot \mathbf{u}) \right) + \frac{\epsilon^2 Pr Ra}{\alpha} (\rho - 1) \frac{\hat{\mathbf{g}}}{|\hat{\mathbf{g}}|}, \quad (6)$$

$$\rho \frac{\partial \theta}{\partial t} + \rho \mathbf{u} \cdot \nabla \theta = \epsilon \nabla^2 \theta + \frac{\epsilon^{-1} \omega}{1 - \alpha}, \quad (7)$$

$$\rho \frac{\partial Z}{\partial t} + \rho \mathbf{u} \cdot \nabla Z = \epsilon \nabla^2 Z, \quad (8)$$

$$\rho = \left(1 + \frac{\alpha}{1 - \alpha} \theta \right)^{-1}, \quad (9)$$

which are subject to the boundary conditions

$$\theta = 0, \quad Z = y, \quad u = v = 0 \quad \text{at } y = 0, y = 1, \quad (10)$$

$$\theta = 0, \quad Z = y, \quad \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0 \quad \text{at } x = \infty, \quad (11)$$

$$\frac{\partial \theta}{\partial x} = \frac{\partial Z}{\partial x} = u = \frac{\partial v}{\partial x} = 0 \quad \text{at } x = 0, \quad (12)$$

and suitable initial conditions.

Here

$$\epsilon = \frac{l_{Fl}}{L} = \frac{D_T/S_L^0}{L} \quad (13)$$

is the flame-front thickness l_{fl} measured against the unit length L . The remaining non-dimensional parameters are

$$Ra = \frac{g(\hat{\rho}_u - \hat{\rho}_{ad})L^3}{\nu \hat{\rho}_u D_T}, \quad \text{and} \quad Pr = \frac{\nu}{D_T},$$

which are the Rayleigh number and the Prandtl number, respectively, where ν is the kinematic viscosity $\nu = \mu/\hat{\rho}_u$. Note that ϵ can be related to a Damköhler number (such as the one used in [35]) by

$$Da = \frac{1}{\epsilon^2(1 - \alpha)}. \tag{14}$$

The non-dimensional reaction rate is

$$\omega = \frac{\beta^3}{4} \rho_{y_F} \rho_{y_O} \exp\left(\frac{\beta(\theta - 1)}{1 + \alpha(\theta - 1)}\right), \tag{15}$$

where y_F and y_O are given in terms of Z in (3). We fix $\alpha = 0.85$ for simplicity [33]. The non-dimensional problem is now fully formulated and is given by Eqs. (5)–(15). The non-dimensional parameters in this problem are α , β , Pr , Ra , ϵ and S . In the next section we solve this problem numerically, with particular emphasis on the effect of ϵ , α and Ra for realistic values of Pr and β . We neglect the effects of heat-loss, differential diffusion and the stoichiometric coefficient S ; these aspects of the problem would be interesting to investigate in future studies but are ignored here for the sake of simplicity and clarity.

2.2. Numerical procedure

Results are obtained by numerically solving the problem (5)–(15) in the finite-element package Comsol Multiphysics. This has been extensively tested in combustion applications, including our previous publications on diffusion flames [35] and triple flames [33], where more detailed descriptions of the numerical procedure can be found. The domain is covered by a grid of approximately 200,000 triangular elements, with local refinement around the reaction zone. Solutions have been tested to be independent of the mesh and the size of the domain. Due to space limitations, only a fraction of the obtained solutions are given here; further solutions can be found in [37]. In all simulations we fix $\beta = 10$, $Pr = 1$ and $S = 1$.

3. Results

3.1. Flame tubes

To provide a criterion for the thermal energy required for initiation of triple flames, we first investigate steady, planar, non-propagating solutions of Eqs. (5)–(15), which we refer to as *flame tubes*. We

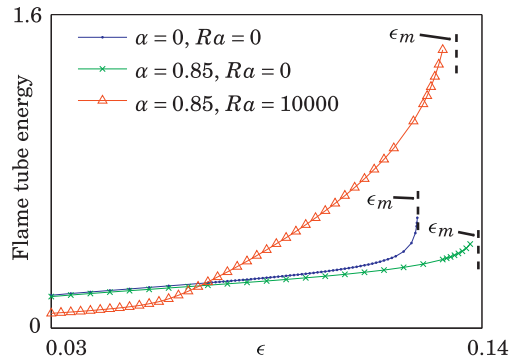


Fig. 2. Flame tube energy E versus ϵ for selected values of α and Ra . Also indicated on the figure for each case is the value of ϵ at which the triple flame propagation speed is zero, denoted ϵ_m . Flame tube solutions are not found for $\epsilon > \epsilon_m$.

define the thermal energy E of a planar flame per unit depth by

$$E = \int_{x=-\infty}^{\infty} \int_{y=0}^1 \theta \, dy \, dx = 2 \int_{x=0}^{\infty} \int_{y=0}^1 \theta \, dy \, dx. \tag{16}$$

Flame tube solutions are found not to exist for $\epsilon > \epsilon_m$, where ϵ_m is the value of ϵ above which positively propagating triple flames do not exist. The critical Damköhler number, below which flame ignition is not expected to be successful, can be found by inserting ϵ_m into Eq. (14). It should be noted that technically flame tube solutions also do not exist in the asymptotic limit $\epsilon \rightarrow 0$. This can be seen by considering the problem (5)–(15) in the limit of infinite activation energy and taking $\epsilon \rightarrow 0$. The problem reduces to finding stationary, two-dimensional tubes in a homogeneous mixture; such a problem is known to have no solution. This is because the leading order term for the temperature is governed by the cylindrically symmetrical Laplace equation in the unburnt gas, whose only solution that satisfies the boundary conditions in the far field is $\theta = 0$. This, of course, is a contradiction since the temperature should be given by $\theta = 1$ at the reaction sheet.

We plot the flame tube energy E versus ϵ for selected values of α and Ra in Fig. 2. It can be seen that E monotonically increases with increasing ϵ in all cases. When thermal expansion is present but gravity is not taken into account, the flame tube energy for each value of ϵ is lower than in the constant density case $\alpha = 0$, $Ra = 0$. It can be seen that the flame tube energy increases sharply as ϵ approaches ϵ_m .

Reaction rate contours of the flame tubes can be seen by examining Figs. 3 and 4 (discussed in more detail in the next section), which show the flame tubes used as initial conditions for the unsteady calculations of

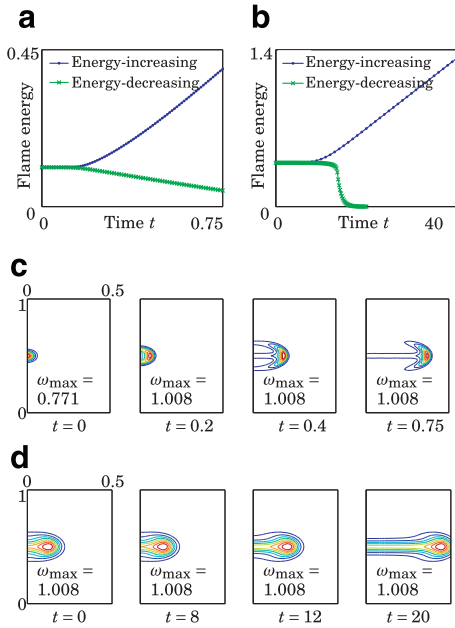


Fig. 3. Transient evolution of triple flames for $\alpha = 0$, $Ra = 0$. Flame energy E is plotted for (a) $\epsilon = 0.05$ and (b) $\epsilon = 0.12$, after a small energy-decreasing or energy-increasing perturbation is added to the unstable flame tube solution. Reaction rate contours (equally spaced up to ω_{\max}) are plotted for triple flames with energy-increasing perturbations for (c) $\epsilon = 0.05$ and (d) $\epsilon = 0.12$ (flame tube solutions shown at $t = 0$).

triple flames. In situations where $Ra = 0$, no flow is induced by the flame tubes, which are symmetric about the line $y = 0.5$. Therefore, in this case the flame tube energy can be found without solving the Navier–Stokes equations by solving the steady form of Eqs. (7)–(15) with $\mathbf{u} = \mathbf{0}$. When $Ra > 0$, flow is induced due to the temperature gradient between the hot flame tube and the cold fluid at $x = \pm\infty$, causing a vortex which deforms the flame tube (Fig. 4d).

3.2. Triple flame evolution

In this section, we perform time-dependent simulations of triple flames. As initial condition, we use a flame tube with a small initial perturbation that either increases or decreases the thermal energy of the flame tube; the perturbations are referred to as “energy-increasing” or “energy-decreasing” perturbations, respectively, throughout the rest of this section. The perturbations, which have order of magnitude 10^{-3} , are added to the stationary temperature field in a region surrounding the midpoint of the domain, with size of the order of magnitude of the stationary tube. For such perturbations, it has been checked that it is the sign of the total perturbation energy that determines flame evolution. It is worth noting that true tran-

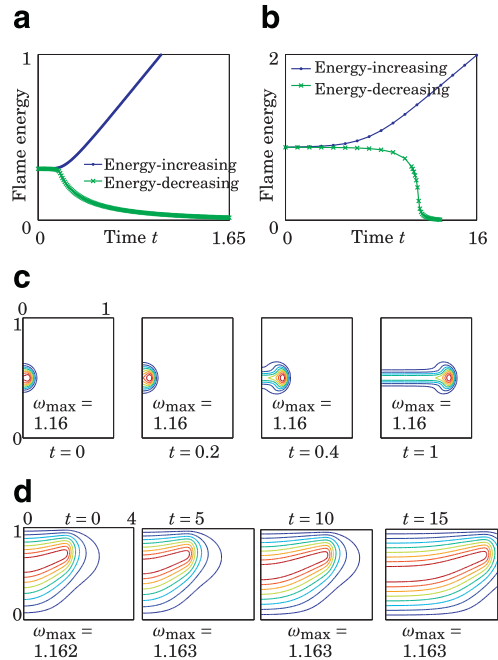


Fig. 4. Transient evolution of triple flames subject to thermal expansion and gravity. Flame energy E is plotted for (a) $\epsilon = 0.12$, $\alpha = 0.85$, $Ra = 0$ and (b) $\epsilon = 0.1325$, $\alpha = 0.85$, $Ra = 10,000$, after a small energy-decreasing or energy-increasing perturbation is added to the unstable flame tube solution. Reaction rate contours (equally spaced up to ω_{\max}) are plotted for triple flames with energy-increasing perturbations for (c) $\epsilon = 0.12$, $\alpha = 0.85$, $Ra = 0$ and (d) $\epsilon = 0.1325$, $\alpha = 0.85$, $Ra = 10,000$ (flame tube solutions shown at $t = 0$).

sient ignition will be strongly dependent on initial conditions; for example, the growth time of time-dependent flame ball solutions after perturbations has been shown to be comparable to the growth rate of a linear stability analysis [3]. However, in this study we are concerned with testing the effect of adding or subtracting energy from flame tube solutions, to identify a possible criterion for the ignition energy of triple flames; instantaneous perturbations to the steady flame tube solutions are sufficient for this purpose.

We begin with triple flame initiation and evolution in the constant density approximation $\alpha = Ra = 0$ (Fig. 3). Plotted in the figure are the flame energy E and reaction rate contours for flame tubes subject to either an energy-increasing or an energy-decreasing perturbation, for various values of ϵ . These figures show that, if an energy-increasing perturbation is added, the flame tube solution will evolve in time into a steadily propagating triple flame. This happens on a much shorter timescale for lower values of ϵ . If an energy-decreasing perturbation is added, the flame extinguishes and the flame energy decays to zero.

Next we investigate the effects of thermal expansion and gravity on triple flame initiation and evolution (Fig. 4). As in the constant density case, an energy-increasing perturbation to a flame tube solution leads to the steady propagation of a triple flame and an energy-decreasing perturbation leads to extinction. Thermal expansion induces a shear flow ahead of the flame due to the symmetry boundary condition applied at $x = 0$ (not shown due to space limitations). The expanded gas pushes the triple flame, increasing its propagation speed. This is akin to the propagation of a 3D spherically expanding flame in the presence of thermal expansion. When gravity is present, a vortex is induced ahead of the flame by the temperature gradient between the unburnt gas ahead of the flame and the flame-front, causing the triple flame to curve (Fig. 4d); the shape of the triple flame in this case agrees with a previous study of steady triple flames subject to buoyancy effects [33].

In all cases it has been found that energy-increasing perturbations to flame tubes lead to the evolution of triple flames, and energy-decreasing perturbations lead to extinction. Therefore we conclude that the energy of these flame tube solutions may be used as a criterion for the *ignition energy* per unit depth of a planar triple flame. In all simulations, we have observed that the stationary flame tube solutions are unstable irrespective of the amplitude of the perturbation added. This is in line with physical expectations of the solutions to be linearly unstable.

4. Conclusion

In this paper, we have described steady, planar solutions in the mixing layer which we have referred to as “flame tubes”. The solutions are unstable and we have shown that perturbations increasing the thermal energy of flame tubes lead to triple flame propagation, while perturbations decreasing the thermal energy lead to extinction. Therefore we have concluded that the thermal energy of flame tube solutions may provide a possible criterion for the ignition energy per unit depth of planar triple flames via a cylindrical ignition kernel, analogous to spherical flame balls for spherically expanding flames. A cylindrical ignition kernel could be generated, for example, by a hot wire. In particular, we have found that a criterion for the ignition energy of triple flames can be given without solving the Navier–Stokes equations, if gravity is not present. We have also shown how triple flames evolve after initiation from flame tubes, including the combined effects of thermal expansion and gravity.

An extension of the present study would be to investigate flame tubes in other mixing layers, such as the counterflow configuration. Such structures could provide a corresponding criterion for the ignition energy of triple flames in that configuration.

In particular, it would be interesting to examine the effect of strain on such structures, given that previous studies have found a critical strain rate above which forced ignition is impossible [38]. Future studies will also investigate the effect of different initial conditions on the energy required for triple flame initiation and the transient dynamics of triple flames in situations where the planar diffusion flame is unstable due to gravitational effects. It would also be of interest to study the stability of flame tubes in more detail, including identifying situations in which flame tubes are stable.

Research Data

All relevant research data is contained within the figures in the publication.

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