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The influence of spatial discreteness on the thermo-diffusive instability of flame propagation with infinite Lewis number

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Abstract

The dynamics of flame propagation in systems with infinite Lewis number and spatially discretized sources of heat release is examined, which is applicable to the combustion of suspensions of fuel particles in air. The system is analyzed numerically using a one-dimensional heat equation with a source term for the reaction progress variable, which is specified to have zero diffusivity, and the model reveals a spectrum of flame-propagation regimes. For the case of a switch-type reaction rate and homogeneous media (continuous regime), the flame propagates steadily at a velocity in agreement with analytical solutions. As the sources are spatially concentrated into δ-function-like sources, propagation approaches the discrete regime with a fixed period between ignition of the sources, for which an analytic solution is also available for validation. When the source term is governed by an Arrhenius rate and the activation energy is increased beyond the stability boundary, the flame begins to exhibit a long-wavelength (4–5 times the thermal flame thickness) oscillation characteristic of the thermo-diffusive instability, in good agreement with prior stability analysis. When spatial discreteness is introduced, a competition is observed between the long-period oscillations of the thermo-diffusive instability and the pulsations associated with the rapid heat release of the concentrated sources. Interestingly, the presence of spatial discreteness is able to excite higher modes (period doubling and chaotic solutions) of the thermo-diffusive instability, suggesting that the introduction of discreteness may have an influence qualitatively similar to that of increasing activation energy. Relevance of the model parameters to experimental systems is then discussed.

Keywords: Flame instability; Lewis number; Particulate; Heterogeneous combustion; Pulsating flames

1. Introduction

In many practical applications, incomplete mixing of fuel with oxidizer can result in the creation of inhomogeneous mixtures, wherein

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pockets of mixture that are able to burn alternate with regions that are effectively inert and flame propagation is not possible. Such systems may be created, for example, in the eddies of turbulent jets of fuel (gaseous or solid particulate) into an oxidizing atmosphere [1,2], incomplete blending of powdered reactants in pyrotechnic and Self-propagating High-temperature Synthesis (SHS) compositions, or produced intentionally, such as in pyrotechnic delay trains, in order to achieve very low burn rates [3]. Despite the presence of effectively inert gaps, many such systems can burn to completion via molecular transport through the inert regions, providing a delivery mechanism of the "ignition signal" between neighboring combustible pockets. In the case of a three dimensional system of randomly positioned pockets, an external observer may even observe what appears to be a continuous flame but may manifest some unusual propagation characteristics. To date, there have been a few attempts to study such systems, with the models that have appeared neglecting to consider the thermal gradients or flames inside the reactive pockets [4-6]. In some cases, this assumption is justified, such as in models of flame propagation in systems with highly spatially discrete sources. Such models are appropriate for treating systems of solid fuel particulates in suspension in gaseous oxidizer [4,6], since in these systems the particle size is negligible in comparison to the inter-particle spacing. The present study considers a more general case where the reactive pockets are not necessarily of negligible size.

In this paper, we consider spatially inhomogeneous, one-dimensional systems wherein reactive layers alternate in a regular array with layers that are nonreactive. For simplicity, we assume the diffusivity of the rate-limiting component is zero, as would be the case for a fuel-lean suspension of solid fuel in an oxidizing atmosphere where the particles remain in the condensed phase during the entire reaction and the global diffusion of the oxidizer is negligible, or in solid pyrotechnic or SHS compositions. Due to zero mass diffusivity, the distribution of fuel does not significantly change during the passage of the flame, which must rely solely upon thermal conduction in order to propagate. The regularly spaced suspension of nonvolatile fuel particles described by an ignition temperature "switch" was investigated in [4,5], and this scenario can be considered as the limiting, asymptotic case since the particles can be represented as spatial δ-functions. An analytic solution for flame propagation is available for this case [4], and thus can serve as verification of the numerical simulations presented in the current paper in the limit of highly discrete, reactive layers.

With the assumption of zero mass diffusivity of the rate limiting component, the Lewis number for the reactive system approaches infinity (Le $\rightarrow \infty$), and as a result, flame propagation in a system that is homogeneous (i.e., continuum case) and described by an Arrhenius reaction rate is inherently unstable, as shown by Shkadinskii et al. [7]. Unlike mixtures with Le less than unity that exhibit a multidimensional cellular instability [8], the limit of large Le results in a one-dimensional oscillatory instability of the flame front for sufficiently large values of activation energy [9,10]. The flame front oscillations result in a spatial wavelength attributed to this inherent instability for the case of a homogeneous media. In the present study, the existence of alternating layers of reactive and inert media imposes an additional length scale to the problem, and the flame is expected to exhibit large pulsations as it traverses these intrinsic inhomogeneities in the system. In this study, the interplay between the oscillatory thermo-diffusive instability and the pulsating nature of flame propagation due to the alternating reactive layers is investigated as a function of the relative magnitude of these length scales, and as explored in detail below, displays a rich spectrum of different front dynamics.

2. Problem description and numerical method

2.1. Problem description

This problem is governed by the one-dimensional heat diffusion equation for temperature T with a reaction source term and an equation tracking the reaction progress variable, C. The dimensionless form of the governing equations is as follows,

$$T_t = T_{xx} + \frac{R(T,C)}{\Gamma}, \qquad C_t = -R(T,C) \tag{1}$$

For the switch-type model,

$$R(T,C) = \begin{cases} 0 & T < T_{\mathrm{ig}} \text{ or } C = 0 \\ 1 & T \geq T_{\mathrm{ig}} \text{ and } C > 0 \end{cases} \tag{2}$$

and for the Arrhenius reaction rate,

$$R(T,C) = C(1-\sigma)\mathrm{Exp}(-N/T) \tag{3}$$

The variables are non-dimensionalized as follows (note that tilde "$\sim$" indicates dimensional quantities). Time is $t = \tilde{t}/\tilde{t}_{\mathrm{r}}$ where $\tilde{t}_{\mathrm{r}}$ is the characteristic reaction time. Note that, for the Arrhenius reaction rate, $\tilde{t}_{\mathrm{r}}$ is the inverse of the pre-exponential (or collision frequency) factor ($\sim 1/\mathrm{s}$). The spatial coordinate is $x = \tilde{x}/\sqrt{\tilde{\alpha}\tilde{t}_{\mathrm{r}}}$ where $\tilde{\alpha}$ is the thermal diffusivity. C is the dimensionless reaction progress variable representing the concentration of reactant. The adiabatic flame temperature is $\widetilde{T}_{\mathrm{f}} = \widetilde{T}_0 + \tilde{Q}/\tilde{\rho}\tilde{c}_{\mathrm{p}}$ where $\widetilde{T}_0$ is the initial temperature of the unburnt mixture and $\tilde{Q}$ is the average volumetric energy density of the system. For the switch-type model, temperature is $T = (\widetilde{T} - \widetilde{T}_0)/(\widetilde{T}_{\mathrm{f}} - \widetilde{T}_0)$,