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Instability growth rates in hydrofluorocarbon/air flames: analysis of the Rayleigh-Taylor instability

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Abstract: Hydrofluorocarbons (HFC), which are mildly flammable and pose potential fire risks, have received greater attention as a viable low global warming potential alternative to traditional refrigerant and fire-suppressant compounds. However, the reactivity of these compounds can be exacerbated under certain conditions, with buoyancy-induced instability growth promoting flame acceleration and substantially increasing flame speeds of HFC/oxidizer deflagrations. Therefore, the flame acceleration of HFC/oxidizer deflagrations must be investigated to properly assess the flammability characteristics of these compounds. This study investigates the effect of the Rayleigh-Taylor instability on instability growth rates during the linear regime. To this end, simulations were performed tracking the growth of instabilities caused by an initial disturbance in the flame front, from which dispersion relations were derived for R-32/air mixtures varying the gravitational acceleration.

Keywords: Hydrofluorocarbons, Rayleigh-Taylor instability, Instability growth, Dispersion relation

1. Introduction

In the last decade, several major international conferences, such as the Twenty-Eighth Meeting of the Parties to the Montreal Protocol have promoted the adoption of refrigerants with both lower ozone-depletion potential (ODP) and lower global warming potential (GWP) [1]. A group of hydrofluorocarbon (HFC) compounds have been identified with viable ODP and GWP characteristics [2]. However, this particular group of HFCs are mildly flammable, obeying the general inverse relationship between flammability and GWP [2]. As these mildly flammable HFCs pose potential fire risks, the flammability and reactivity of these compounds need to be quantified in order to establish proper safety metrics [3]. The flammability characteristics of these candidate HFCs have been assessed through the laminar flame speed S_u^0, a fundamental combustion parameter often used for kinetic model validation and turbulent combustion scaling [3]. However, previous studies have shown that the reactivity of these compounds can be exacerbated under certain conditions [4]. Papas et al. [4] showed that a confined volume can significantly increase the severity (flame propagation speed and overpressure rise) of turbulent deflagrations of R-32 and R-1234yf mixtures. In addition, their experimental tests demonstrated the importance of buoyancy effects for deflagrations propagating in vertical spaces [4]. As weakly propagating HFC/oxidizer flames are particularly susceptible to buoyancy effects, the growth of the Rayleigh-Taylor instability may contribute to flame acceleration, leading to overall consumption speeds (S_c) several times that of S_u^0. Therefore, in addition to accurately quantifying S_u^0, the flame acceleration of HFC/oxidizer flames must be investigated to properly assess the flammability characteristics of these compounds.

Flame acceleration caused by the growth and non-linear evolution of combustion instabilities can substantially change flame dynamics, total heat release rates, and S_c [5,6]. In premixed flames propagating with a subsonic velocity, flame front instability is caused by three basic types of phenomena: hydrodynamic, body-force, and thermal-diffusive effects [5-8]. The hydrodynamic effect is caused by thermal expansion through the flame surface. As all premixed flames are highly exothermic, resulting in large thermal expansion ratios, the hydrodynamic effect exists in all premixed flames and cannot be neglected. In addition, the body-force effect is caused by the difference in density between the upper and lower fluids caused by thermal expansion. This effect has a stabilizing influence on downward propagating flames and a destabilizing influence on upward propagating flames. Finally, the thermal-diffusive effect is caused by the preferential diffusion of mass versus heat. This effect has a stabilizing influence when the Lewis number (Le) of the deficient reactant is greater than unity and a destabilizing influence when Le of the deficient reactant is lower than unity.

Because of intrinsic instability, a perturbation in a premixed flame can grow, eventually resulting in a cellular flame. The initial disturbance of a flame front can be modeled as a weak harmonic perturbation $F(x)$ with initial amplitude A_0 and wavenumber k [5-8]. By varying the wavelength of the perturbation λ_y, one can obtain the dispersion relation between the exponential growth rate σ and k during the linear regime, during which the disturbance amplitude grows with constant σ. Dispersion relations show the magnitude of σ along the range of unstable k during the linear regime, from which the relative magnitude of σ can be used to predict trends during the long-term non-linear regime. Previous studies have shown that the maximum growth rate σ_{max} may have a direct correlation with S_c and the extent of flame acceleration in the non-linear phase [7,9-11]. In particular, the critical wavelength $\lambda_{y,max}$ (i.e., k_{max}) corresponding to σ_{max} has been shown to be an important length scale for instability growth in the non-linear regime [7,9].

The linear analysis of Darrieus and Landau (DL) is a fundamental study which acknowledged the fundamentals of flame instability [5,6]. This analysis assumed an infinitely-thin flame front and constant pressure conditions for flames propagating with speeds sufficiently small compared with that of the speed of sound. The DL analysis predicted that the hydrodynamic instability was unconditionally unstable for all λ_y, in which the growth rate of the DL instability σ_{DL} increased with increasing k. However, the applicability of the DL solution was found to be limited to sufficiently small k due to the underlying assumptions. Specifically, by assuming an infinitely thin flame front, the DL solution neglects the interaction of thermal-diffusive effects with the hydrodynamic instability. Theoretical analysis performed by Clavin [5] revealed that the analysis of the DL instability ceases to be valid at small λ_y, when the scale of wrinkling becomes comparable to the flame thickness. As the curvature of the perturbed flame front produces transverse fluxes of energy and species, the gradients of these fluxes modify the local internal structure of the wrinkled flame and local reaction rates, leading to values for S_c which differ from S_u^0 [5]. Thermal-diffusive effects were found to cause a relaxation or growth in the overall instability amplitude growth rate based on the Le of the mixture, where a growth is found in mixtures with $Le < 1$ leading to the thermal-diffusive (TD) instability [5]. In addition, for a flame propagating upwards, body-force effects due to gravity produce a destabilizing effect for large λ_y (small k), known as the Rayleigh-Taylor (RT) instability [5]. When combined with the DL and

TD instabilities, the RT instability can substantially increase σ and further broaden the unstable range of the dispersion relation. Therefore, quantifying the interaction of the various instabilities is essential for accurately computing the dispersion relation and predicting unstable conditions.

However, there have yet to be studies which quantify flame acceleration due to the various instabilities for mildly reactive HFC/air flames, in which growth rates are exacerbated by the RT instability due to their characteristically low values for S_u^0 (~3-7 cm/s). Therefore, there is a need to study the combined effects of the various instabilities on flame acceleration in mildly reactive HFC/air flames.

2. Methods

DNS studies using a 2-D rectangular geometry will be used to study the growth and interaction between DL, TD, and RT instabilities in slowly-propagating HFC/air flames. PeleLMeX [12], an open-source software based on the low Mach number reactive flow algorithm of PeleLM and built upon the block-structured adaptive mesh refinement (AMR) framework of AMReX, will be used to perform the simulations. A schematic of the simulation is provided in Figure 1. Periodic boundary conditions (BCs) are used in the transverse (x) direction, while inflow (Dirichlet) and outflow (Neumann) BCs are used in the main flow direction (y). The inflow gas velocity is set as the S_u^0 of the unburned gas mixture. The initial condition is a freely propagating laminar flame profile (i.e., a Cantera freely propagating flame solution obtained from PelePhysics functionalities using the R-32 chemical model developed by Babushok et al. [3]) perturbed by a harmonic disturbance of wavelength equal to the length of the domain in the transverse direction (L_x). The wavelength of the harmonic disturbance will then be varied by changing L_x for the same unburned mixture conditions. Simulation results will be post-processed to derive the flame front harmonic profile, defined by the location of max. heat release rate (HRR) along the transverse direction. The amplitude of the flame front harmonic $A(t)$ will then be evaluated as the difference between the right antinode and the initial node position. Convergence tests were conducted to determine proper values for parameters controlling grid refinement and time step size to allow for converged solutions for $A(t)$. Subsequently, $\partial(\ln A(t))/\partial t$ will be plotted as a function of t, from which σ is determined for the region of linear growth, marked by a plateau of constant σ after an initial transient. The dispersion relation will then be generated for several cases in which the magnitude of the gravitational acceleration (G) will be varied in terms of the actual acceleration due to gravity (g).

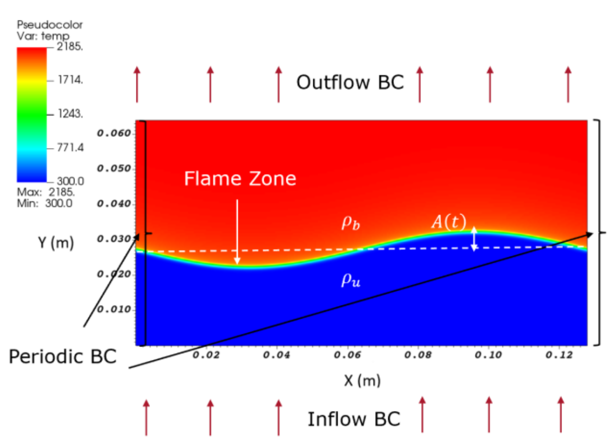

Figure 1: Schematic of simulated 2-D R-32/air flame with harmonic disturbance.

3. Results and Discussion

Transient, 2-D R-32/air flame simulations at ambient conditions (1 atm and 298 K) were performed varying the gravitational acceleration. An equivalence ratio (φ) of φ = 1.4 was used for all cases in this study, with an S_u^0 of ~4.9 cm/s at ambient conditions. This value for φ was chosen because the R-32/air mixture was found to be thermal-diffusively "neutral", with a Markstein number (Ma) and effective Lewis number of approx. 0.0 and 1.0, respectively. Therefore, the dependence of the growth rate on the coupling of the DL and RT instabilities could be isolated. Exponential growth rates during the linear regime were computed for various wavelengths, and the dispersion relation for several values of G are shown in Figure 2. In addition, Figure 2 shows the dispersion relation for the case neglecting the gravitational body force (G=0). The growth rate σ and wavenumber k are non-dimensionalized by S_u^0 and the flame thickness l_f, as is often done in the literature.

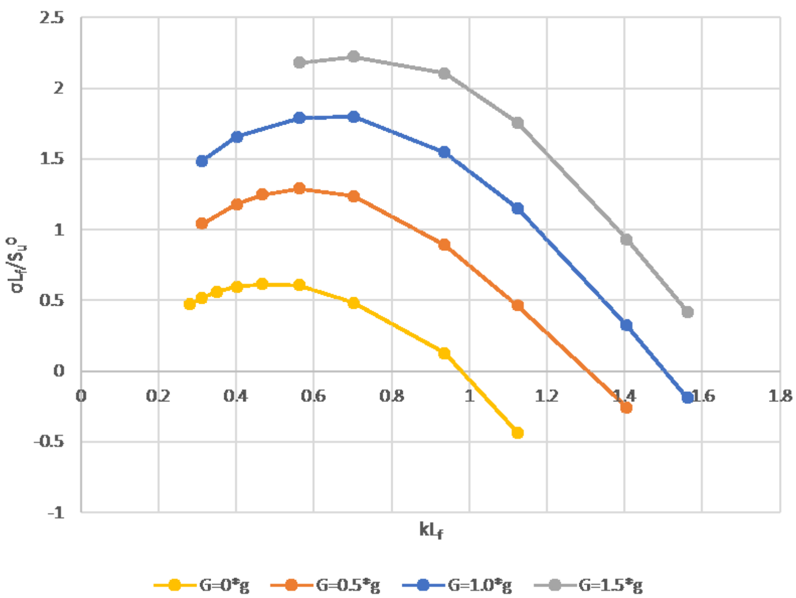

Figure 2: Dispersion relation (non-dimensional growth rate vs. non-dimensional wavenumber) for R-32/air flame front varying gravitational acceleration.

The magnitude of σ_{max} and the range of unstable wavenumbers (positive σ) increases with increasing G, showing the influence of the RT instability on the overall instability growth. The critical wavenumber (k_{max}), corresponding to σ_{max}, appears to slightly increase with increasing G. Furthermore, the relationship between σ_{max} and G appears to follow a square root relation, similarly to the classical RT instability growth rate (σ_{RT}) [5].

4. Conclusions

The growth rates of flame front instabilities were determined in the linear regime for various wavelengths/wavenumbers. A dispersion relation for a rich R-32/air flame at ambient conditions was derived varying the gravitational acceleration. The RT instability, whose contribution to the instability growth depends on the gravitational acceleration, is shown to cause a considerable increase in the maximum growth rate and range of unstable wavenumbers in R-32/air flame fronts. As the maximum growth rate is closely correlated with S_c and the extent of flame acceleration in the non-linear phase, the RT instability is predicted to contribute significantly to flame acceleration in R-32/air flame fronts.

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