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Large eddy simulation of combustion instability in a tripropellant air heater

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ABSTRACT

This research is motivated by the issue associated with high frequency combustion instability. Large eddy simulation was performed to investigate spontaneous combustion instability in an air/LO_2/C_2H_5OH tripropellant air heater. The simulation predicts self-excited transverse oscillations. Overall behavior of combustion instability including pressure time histories, mode shapes, Rayleigh index and unsteady response of the injector were studied in detail. Special emphasis was given to the flame behavior, droplet trajectories, pressure evolutions, and formation of large-scale vortical structures during combustion instability in present air heater. Furthermore, in contrast to previous investigations, a new process is identified in the simulation that may feed energy into the acoustic mode and drive combustion instability.

1. Introduction

Development and characterization of future high speed/hypersonic flight vehicles will require advancements in ground test facility technology (such as air heater (AH)), including the capability to conduct aeropropulsion testing with air as the test medium at Mach number, total temperature, components and pressures that properly simulate the stagnation conditions associated with high speed flight through the earth's atmosphere [1–4]. In general, liquid rocket engine (LRE) technology is applied to meet these requirements by burning little fuel and heating up a large amount of air. For AH, high frequency combustion instability is considered as a major challenge. When it occurs, the pressure fluctuates, which can introduce large thermal and mechanical stresses in the combustor, resulting in decreased performance, unacceptable vibrations or even engine failure [5–7].

To date there is no methodology to reliably predict combustion instability a priori in design of an engine, and only the mechanisms for sustaining high frequency combustion instability are understood well can we suppress it effectively. Thus, these topics are of great concern to the AH community. Thanks to recent advancements in computer capabilities and the dramatic progress in the field of computational fluid dynamics (CFD), numerical simulation of unsteady three dimensional reacting flowfields has emerged as a method of analysing combustion instability mechanisms. Many past studies of combustion instability simulation are based on response function method. With aid of this method, combustion instability can be excited and sustained. Smith et al. [8,9] and Sisco et al. [10,11] conducted extensive numerical studies of acoustics in a rocket combustor with this response function method. Grenda et al. [12,13] analysed combustion instability in LRE with this method. However, this method requires the combustion response function to represent the mechanisms for coupling heat release to the acoustic modes, unfortunately, we cannot get a general theory to design such response function. Recently, dynamics of flame under acoustic forcing are extensively being investigated, including H_2/O_2 flame [14–17], and CH_4/O_2 flame [18,19], indeed, these studies can provide considerable insight into the understanding of physical mechanisms responsible for combustion instability. However, it is difficult to design the frequency, position and methodology of the acoustic forcing, which can notably affect the results. For example, Hakim et al. [19] demonstrated that when the flame is modulated at a frequency close to the natural frequency of the oxygen jet the flame motion may be assimilated to that of a flag flapping in the wind, when the flame is modulated at a higher frequency, it features a corrugated surface extending in the axial direction and executing a bulk motion in the transverse direction with no large scale deformation. Moreover, in real combustor, combustion instability appears spontaneously without artificial acoustic forcing. Accordingly, great prominence is put on employing a complete computational model that automatically includes the coupling between the chamber acoustic modes and the propellant combustion process so that combustion

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instability can be excited spontaneously and self-sustained like the situation in real engine. The present paper describes a large eddy simulation (LES) of spray combustion in an air/LO_2/C_2H_5OH tri-propellant AH. Unlike most previous work [20–23], here combustion instability is excited spontaneously and self-sustained.

Though recently reported experimental measurements in LRE [24–27] have provided precious information on dynamics of flame submitted to acoustic forcing, combustion instability in AH is still poorly understood, with considerable argument as to the mechanisms that lead to disturbance growth and/or sustained oscillations. To address this issue, present study tries to identify possible combustion mechanisms using LES. To the authors' knowledge, this represents the first reported attempt at using CFD simulation to capture spontaneous combustion instability and identify its sustaining mechanisms in AH.

The present project aims at advancing the state of the art of combustion instability by making use of LES. It has three objectives: (1) Capture spontaneous combustion instability in AH. (2) Analyse unsteady behaviors in the fast transient spray-combusting flows and dynamics of spray droplets during spontaneous combustion instability. (3) Identify sustaining mechanisms of combustion instability in present AH.

2. Brief description of the computational model

Numerical simulations performed in this paper were carried out using the density-based solver in the commercial code ANYSYS [28]. Investigation of combustion instability in a rocket has been performed successfully utilizing this code [29].

2.1. Gas phase

The gas phase is simulated in an Eulerian frame by solving transport equations for a compressible, turbulent, and reactive mixture. The density-weighted filtered governing equations, with the two-way coupling between the gas and liquid phase included, can be written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = \widetilde{\dot{\rho}_s} \tag{1}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) = \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_j} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \widetilde{F_{s,i}} \tag{2}$$

$$\frac{\partial(\bar{\rho}\tilde{E})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{E} + \bar{p})\tilde{u}_i}{\partial x_i} = -\frac{\partial(\bar{q}_i + H_i^{sgs})}{\partial x_i} + \frac{\partial\left[(\bar{\tau}_{ij} - \tau_{ij}^{sgs})\tilde{u}_j\right]}{\partial x_i} + \bar{S}_h + \widetilde{Q_s} \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{Y}_m) = \frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc}\frac{\partial \tilde{Y}_m}{\partial x_j}\right) - \bar{w}_m - \frac{\partial g_j}{\partial x_j} + \widetilde{S_{s,m}} \tag{4}$$

where t is the physical time, ρ is the density, x_i and u_i are the position and velocity respectively for direction i ($i = 1, 2, 3$ represents for the Cartesian coordinates x y z respectively), p is the pressure, E is the total energy, τ_{ij} is the viscous stress, q_i is the heat flux vector, g_j is the species flux vector, and Y_m is the species mass fraction. The over bars and tildes represent, respectively, spatially filtered and density weighted filtered values with a filter width $\Delta_f \equiv (\Delta x \Delta y \Delta z)^{1/3}$, which is based on local grid (Δx, Δy, Δz). The subgrid terms, denoted with superscript (sgs), represent the small-scale effects upon the resolved-scales in the form of additional stresses and fluxes. $\bar{S}_h$ is the gas source term due to chemical reaction. Subscript s denotes source terms from dispersed phase and index m for species varies from 1 to $N_{SP} - 1$, where N_{SP} is the total number of species. Coupling between the dispersed phase and the gas phase are provided by the interphase exchange terms or the source terms that appear on the right-hand side of the LES equations ($\widetilde{\dot{\rho}_s}$, $\widetilde{F_{s,i}}$, $\widetilde{Q_s}$, $\widetilde{S_{s,m}}$). For details of the mathematical development, the reader should consult references [30,31].

The sub-grid stress tensor is modeled as

$$\tau_{ij}^{sgs} = \frac{2}{3}k^{sgs}\delta_{ij} - 2\mu_t\tilde{S}_{ij} \tag{5}$$

where resolved strain-rate is given as $\tilde{S}_{ij} \equiv (1/2)\left(\partial\tilde{u}_i/\partial x_j + \partial\tilde{u}_j/\partial x_i\right)$. The subgrid-scale eddy viscosity, μ_t is computed using subgrid kinetic energy k^{sgs} as $\mu_t = C_k\sqrt{k^{sgs}}\Delta_f$, k^{sgs} is obtained by solving its transport equation:

$$\frac{\partial k^{sgs}}{\partial t} + \frac{\partial \tilde{u}_j k^{sgs}}{\partial x_j} = -\bar{\tau}_{ij}\frac{\partial \tilde{u}_i}{\partial x_j} - C_\varepsilon\frac{(k^{sgs})^{3/2}}{\Delta_f} + \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k^{sgs}}{\partial x_j}\right) + \bar{W}_s \tag{6}$$

In the above equations, subgrid kinetic energy k^{sgs} is defined as $k^{sgs} = (1/2)(\widetilde{u_i u_i} - \tilde{u}_i\tilde{u}_i)$. $\bar{W}_s$ is the production/destruction term due to presence of spray. C_k and C_ε are the model constants. σ_k is hardwired to 1. Additional details are given in the cited literature.

Chemical conversion is modeled by a single-step, global reaction:

$$C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O \tag{7}$$

This approach allows global energy-release effects to be included with a minimum number of species equations to be solved. The Arrhenius-based kinetics is applied, which readily incorporates the effects of pressure fluctuations on heat release, an interaction that is imperative for combustion instability.

2.2. Liquid phase

For simplicity, liquid jet breakup and primary atomization are not considered in this paper. Also, no secondary atomization is considered. Instead, a droplet distribution is imposed at the injector. Atomization process of LO_2 and C_2H_5OH jets are modeled as LO_2 and C_2H_5OH droplets respectively by Discrete Phase Model (DPM). In the DPM model, droplets are tracked in a Lagrangian frame. Required information of the surrounding gas for the droplets is provided by the gas code. In turn, gas phase source terms are calculated and passed to the gas code. The models of spray evaporation are described elsewhere [28,30], and therefore only briefly summarized next.

Droplet motion is governed by Eq. (8) (in Cartesian coordinates):

$$\frac{d^2\vec{x}}{dt^2} = \frac{d\vec{u}_P}{dt} = F_D\left(\vec{u} - \vec{u}_P\right) + \vec{g}\cdot\left(1 - \frac{\rho_g}{\rho_P}\right) \tag{8}$$

Instantaneous mass vaporization rate $\dot{m}$ from the droplet surface are calculated using following equation:

$$\dot{m} = k_c \cdot A_P \cdot \rho_g \cdot B_M \tag{9}$$

It is shown that quasi-equilibrium and non-equilibrium models provide different results for gasification of liquid fuel in diffusion combustion. In order to have adequate data for combustion rate of small droplets it is recommended to use the non-equilibrium model [32–34]. However, in the present study, particular attention is given to combustion instability. In addition, it is difficult to apply non-equilibrium model in spray combustion systems involving