Effects of Droplet Size on Hypergolic Combustion of Hydrazine Spray

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1 Introduction

Bipropellant thrusters containing hydrazine (N_2H_4) and nitrogen tetroxide (NTO), in fact the nitrogen dioxide-nitrogen tetroxide ($NO_2-N_2O_4$) equilibrium, are extensively used in space propulsion. Bipropellant systems using N_2H_4/NTO possess the advantage of retaining hypergolic characteristics even at low-temperatures and in vacuum environments. Hence, pulse mode operations, i.e. cyclic operations of the ignition and quenching occurring at time intervals of 10–100 ms, are possible without ignition devices. Furthermore, the hypergolic ignition characteristics of N_2H_4/NTO are important as they have a significant impact on the combustor performance in pulse mode operations, such as the combustion efficiency and stability [1]. However, little is known about the hypergolic ignition and flame structure of N_2H_4/NTO systems because practical bipropellant thrusters are subjected to complicated multi-physics phenomena such as the liquid jet atomization and spray formation [2], the liquid-phase reaction at impinging regions [3], droplet combustions [4], and gas-phase reactions [5], as shown in Fig. 1. Hence, the fundamental sub-processes should still be investigated by experiments and numerical simulations.

In a recent study, the authors of the study [6] previously investigated the hypergolic combustion of the gaseous N_2H_4 /gaseous NTO co-flowing jets by solving the Navier-Stokes (N-S) equations, based

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on the detailed chemical kinetics mechanism proposed by Daimon et al. [9]. It was revealed that the hydrogen abstraction reactions from N_2H_4 by NO_2 preheat the N_2H_4 and NO_2 mixtures and eventually cause the auto-ignition. Furthermore, the flame structure uniquely comprises two types of flames, i.e. the outer diffusion flame and the inner decomposition flame. The diffusion flame comes from the oxidization of N_2H_4 . The decomposition flame is caused by a high rate of heat release of the thermal decomposition of N_2H_4 . The N_2H_4 spray jets in the gaseous NTO flows were also previously simulated to explore the influence of the droplet evaporation [7]. The evaporation largely delayed the auto-ignition because it decreased the temperature of the N_2H_4 vapor and NO_2 mixtures, and it almost terminated the hydrogen abstraction reactions. Besides, the decomposition flame significantly exhibited a sinusoidal behavior which was caused by the local expansion of the N_2H_4 vapor flows. The previous study also suggested the droplet size affects the auto-ignition delay and flame dynamics. To clarify the influence of the droplet size, the present study simulated the N_2H_4 spray jets with various droplet sizes.



Figure 1. Schematics diagram depicting the complicated multi-physics phenomena in the N_2H_4 /NTO bipropellant thrusters.

2 Numerical Method

The governing equations of fluids are the two-dimensional, compressible N–S equations that include the conservation equations of chemical species. In order to avoid the stiffness of the chemical reaction terms, the fluid and chemical reaction terms were solved separately and explicitly with different time steps. More detailed formulae used in the present study can be found in reference [8]. The transport properties of the single component gas and mixtures were calculated in the same manner of the previous study [7]. The detailed chemical reaction mechanism proposed by Daimon et al. [5] with 39 species and 261 reactions was applied to the simulation. Extended Robust Explicit Numerical Algorithm (ERENA) [19] was employed to efficiently conduct the time integration of the chemical reaction equations with the large chemical reaction model. Droplets of sprays were dispersed in the gas phase and were individually tracked based on a Lagrangian framework. The mass, momentum and energy of the evaporated N₂H₄ were given to the gas phase as the source terms of N–S equations. More detailed formulae of the governing equations of dispersed droplets and the evaporation models can be found in references [7, 10, 11].

3 Numerical Conditions

Figure 2 shows a schematic configuration of the spray jets along with a definition of the streamwise (x) and transverse (y) coordinates. Table 1 illustrates the chamber conditions. The dimensions of the computational domain and the injection conditions of the N₂H₄ spray and gaseous NTO, except the droplet size, were set to be same with those used previously under which the auto-ignition was confirmed [7]. There was no velocity difference between the N₂H₄ spray and the gaseous NTO flows; their velocity profiles at the inflow boundary were set to be uniform. The simulations were conducted under six different droplet diameters, as illustrated in Table 1. In each case, the droplets were injected with a constant diameter. The droplet diameter of 30 µm in Case 3 corresponds to that of the previous study [7]. Note that, the N₂H₄ spray was injected at the same mass flow rate in all cases. Table 1 alsho shows the group combustion number (*G*-number) which is given as follows [12];

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$$G = \frac{3}{4} Le \left(2 + 0.552 \operatorname{Re}_{sl}^{1/2} Sc^{1/3} \right) n_T^{2/3} \left(\frac{D}{l} \right)$$
(1)

where *Le* is the Lewis number, n_T is the total number of the fuel droplets and *l* is the mean distance between the fuel droplets. The total number of the droplets was defined as the number of the droplets that exist in an injector-height (7-mm) cube near the injector exit. Because *G*-number in all cases was over 1, the spray combustions were expected to be the external group combustion or external sheath combustion.

The simulations started under the condition that the entire domain fills with the NTO flows at the injection velocities. Notably, no artificial heat source was imposed during the calculations. The computational grid of 651×247 points was also the same previously used [7]. The grid is clustered near the inlet and the jet shear layers with a minimum grid spacing of 0.2 mm.



Figure 2. Computational domain and boundary conditions.

Table 1: Injection conditions.						
		Case 1	Case 2	Case 3	Case 4	Case 5
N ₂ H ₄ spray	Droplet diameter	10 µm	20 µm	30 µm	40 µm	50 µm
	Temperature	320 K				
	Velocity	50 m/s				
	Mass flow rate	0.035 kg/s/m				
	G-number	137	34.3	15.2	8.56	5.48
NTO gas	Pressure	0.01 MPa				
	Temperature	320 K				
	Velocity	50 m/s				
	Mole fractions of NO_2 and N_2O_4	1.000 : 0.000				

4 Results and Discussions

Figure 3 shows the instantaneous contours of the temperature and the mole fraction of N_2H_4 with the droplets in Case 1, 3 and 5 at the moment of the auto-ignition. Note that the mass of the N_2H_4 droplets in cells are not considered in the mole fraction of N_2H_4 . In all cases, the mole fraction of N_2H_4 was relatively high at the end of the N_2H_4 spray core where the dense spray existed. Since the N_2H_4 droplets absorbed the latent heat from the ambient gas during the evaporation process, the temperature decreased in the region where the dense spray existed. Nevertheless, the hydrogen abstraction reactions preheated the N_2H_4 vapor and NO_2 gas mixtures and eventually caused the auto-ignition near the leading edge of the N_2H_4 vapor flows.

The evaporation of the smaller droplets was faster because the surface area of the droplets per unit mass is inversely proportional to the droplet diameter. Hence, the mole fraction of N_2H_4 in the spray



Figure 3. Instantaneous contours of the temperature and mole fraction of N_2H_4 with the droplets at the moments of the auto-ignition in each case.



Figure 4. Ignition delay time with the injection droplet diameter.

regions was higher as the injection droplet size was smaller. Although the evaporation of the smaller droplets was enhanced, the temperature of the N_2H_4 vapor and the NO_2 gas mixtures became lower owing to the evaporation heat and the reaction rates of the hydrogen abstraction reactions became slower. As a result, the ignition delay time was longer as the droplet size was smaller. Figure 4 shows the ignition delay time with the injection droplet diameter of the N_2H_4 spray. The ignition delay time was defined as the time when the maximum temperature in the flow fields exceeds 2000K. In fact, the auto-ignition in the case of the larger droplets of N_2H_4 was faster in the present study.

Figure 5 displays the instantaneous contours of the temperature with the droplets after the flame reached a steady-state. The flame structures in all cases comprised the outer diffusion flames and the inner decomposition flame. As previously discussed [7], the decomposition flames in Case 3 exhibited a sinusoidal behavior. This sinusoidal behavior was induced by the cyclic expansion of the locally auto-ignited gas mixtures of the N_2H_4 vapor and NO_2 . The local auto-ignition of the N_2H_4 vapor and NO_2 gas mixtures was caused by the heat transfer from the flame edges of the outer diffusion flames. Furthermore, the sinusoidal behavior of the decomposition flames was developed by the decomposition of the N_2H_4 vapor which was additionally produced by the droplet evaporation.

In Case 1 and 2 under which the injection droplets were smaller than that of Case 3, the area of the decomposition flames near the flame edge of the diffusion flames was smaller. This is because the temperature of the N_2H_4 vapor was lower and the reaction rates of the thermal decomposition became



Figure 5. Instantaneous contours of the temperature with the droplets after the flame reached a steady state.



Figure 6. Time-averaged profiles of the mole fractions of NH_3 and H_2 at x = 30 cm.

slower. As a result, the sinusoidal behavior of the decomposition flame was less significant. Instead, the outer diffusion flames became thicker. In contrast, the area of the decomposition flames was larger and the outer diffusion flames were thinner in Case 4 and 5. This is because the temperature of the N₂H₄ vapor was higher and the reaction rates of the thermal decomposition were faster. However, the concentration of the N₂H₄ vapor near the flame edges was not high enough to cause the rapid expansion of the auto-ignition of the N₂H₄ vapor and NO₂ gas mixtures because the droplet evaporation was slow. As a result, the sinusoidal behavior of the decomposition flame was less significant than that in Case 3. This result suggested that the droplet size affects the mole fraction and temperature of the N₂H₄ vapor flows, and then they have a large impact on the flame dynamics.

Figure 6 shows the time-averaged profiles of the mole fractions of NH_3 and H_2 at an axial position where the all droplets evaporated. The mole fractions of NH_3 and H_2 correspond to the concentration of the unburned fuels because that of N_2H_4 was almost zero at this position. The mole fraction of NH_3 in Case 3 was obviously lower than those in other cases. This is because the sinusoidal behavior, significantly appeared in Case 3, enhanced the mixing and reaction of the decomposed NH_3 gas. The profiles of the mole fraction of NH_3 were similar in other cases. Generally, the smaller droplets are preferred for the combustion of usual hydrocarbon fuels. However, the finest spray is not always best for the hypergolic propellant combustion.

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5 Conclusions

The N₂H₄ spray jets in gaseous NTO flows were simulated to explore the influence of the droplet size on the auto-ignition and flame dynamics. The ignition delay time was longer as the droplet size was smaller because the smaller droplets enhanced the evaporation and decreased the temperature of the N₂H₄ vapor and NO₂ gas mixtures. Therefore, the key for the fast ignition of the N₂H₄ spray is not to generate the finer spray but to keep the temperature of the N₂H₄ vapor relatively high. As for the flame dynamics, the sinusoidal behavior of the decomposition flames was most significant in Case 3. In the smaller droplet cases, the temperature of the N₂H₄ vapor became too low to induce the cyclic auto-ignition of the N₂H₄ vapor and NO₂ gas mixtures near the flame edges. In the larger droplet cases, the concentration of the N₂H₄ vapor was too low to cause the cyclic auto-ignition. This result suggests that the droplet size affects the mole fraction and temperature of the N₂H₄ vapor flows, and then they have a large impact on the flame dynamics. The sinusoidal behavior of the decomposition flames was that the finest spray is not always best for the hypergolic propellant combustion.

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