

The combustion process of ADN-based liquid propellant in attitude control engine

Liyue Jing, Jialong Huo, Xiaoqing You, Min Zhu
Tsinghua University, Beijing, China

Zhaopu Yao
Beijing Institute of Control Engineering, Beijing, China

1 Introduction

The green propellant or non-toxic propellant is an important research area in propulsion technology. Ammonium dinitramide (ADN, $\text{NH}_4[\text{N}(\text{NO}_2)_2]$) is such a promising green propellant. It is a high-energy inorganic salt that can be used as an oxidizer in both solid and liquid propellant rockets, and has potential to replace ammonium perchlorate because of its high burning rate and chlorine-free combustion. A lot of research on thermal decomposition and combustion of ADN has been reported and reviewed comprehensively by Yang et al in 2005 [1]. These works promoted the development of the ADN solid propellant. The research on ADN-based liquid propellant is much less than that on solid propellant and attracts more attention in recent years. The purpose of developing ADN-based liquid propellant is to replace the toxic hydrazine and a promising way is to dissolve the ADN in a fuel/water mixture. The FOI has developed and tested the FLP series of ADN-based liquid propellants to meet the requirement when stored and used in the spacecraft. One typical composition is 63.4% ADN, 25.4% water, 11.2% methanol (FLP-103) [2].

An important application of ADN-based liquid propellant is to be used in the attitude control engine for a satellite [3]. The thrust chamber is the key part which composes of an injector, a combustion chamber (including a porous media as catalytic bed) and a supersonic nozzle. The physical and chemical processes of ADN-based liquid propellant in the thrust chamber are complicated. The liquid propellant is atomized to small droplets and injected to the combustion chamber. In the preheated catalytic bed, the ADN, fuel and water evaporate from the droplets and react to form small molecule products. The interaction between liquid droplet and porous media enhances the atomization of droplet and contributes the evaporation and combustion due to energy feedback by thermal radiation and conduction through porous matrix [4]. The heat release increases the temperature and pressure in combustion chamber. The internal energy of gas products is transformed to kinetic energy through the nozzle to generate thrust.

The investigations on the combustion process of ADN-based liquid propellant are very limited, and an advanced understanding of this process may promote the application of ADN-based liquid propellant. In this paper, the combustion process of ADN-based liquid propellant in attitude control engine is investigated experimentally and numerically. The propellant composition is 63.4% ADN, 25.4% water and 11.2% methanol.

2 Experiment and modeling setup

In the experiment, the propellant is forced and injected with a mass flow rate of 0.6g/s by high pressure nitrogen. The catalyst bed is preheated to 200°C so that the propellant can be ignited. The pressure of the combustion chamber is measured by the piezometer tube and the temperature of chamber is measured by the nickel chromium-nickel silicon thermocouple. The characteristic species concentrations of CO and NO in the combustion chamber are measured by the TDLAS method.

Many physical and chemical models are employed when simulating the combustion process. The discrete phase model, which is an Euler-Lagrange approach, is employed to simulate the motion of ADN-based droplets in the thruster chamber. For the injection process, the Rosin-Rammler distribution of droplets, which is calculated from the PDA measurement results, is used to describe the performance of injection process and provide the liquid boundary condition for the simulation work. For the evaporation process, the vaporization rate of each component is calculated based on the diffusion-controlled model. Besides, the properties of ADN-based liquid propellant are used during the calculation, including the density, specific heat, thermal conductivity, viscosity, surface tension, latent heat and saturation vapor pressure of propellant. The data of the properties are obtained from experiments and some articles [5]. A solid energy equation is added to simulate the heat transfer through porous media. Considering the enhancement to the evaporation process from porous media, the pseudo-fluid concept is employed so that an external virtual body force is imposed on the droplet motion equation to increase the residence time of droplet in the porous media [6]. Also, an external source is imposed on the droplet energy equation to model the energy feedback from the porous media [7].

A 46 species and 237 reactions detailed chemical mechanism for ADN-CH₃OH gas phase reactions is set up, which is based on the work of Korobeinichev et al [8] and the work of Li et al [9]. Through the DRGEP method, an 18 species and 40 reactions simplified chemical mechanism is obtained and used in the CFD work. Some important reactions are listed Tab.1. Based on the calculated results in Fig.1, we can see that there are two stages of temperature increasing in the ADN-CH₃OH combustion process. The first stage is dominated by the decomposition of ADN. While in the second stage, the oxidization of CH₃OH is important.

3 Results and discussion

Some numerical results are present in Fig.2, including pressure, Mach number, temperature of gas, mole fraction of CO and NO. The pressure is almost uniform in the combustion chamber, and is decreased rapidly across the throat. The highest Mach number is nearly 3 and occurs in the nozzle. Temperature of gas and mole fraction of CO are not uniform in the chamber. The higher values occur near the chamber wall, corresponding to the two jet flow at the inlet boundary. NO almost does not exist in the chamber. The numerical results are compared with the experiment results in Tab.2. The value of pressure, temperature of gas, and mole fraction of species are average values of the slices across the chamber.

The liquid propellant evaporates rapidly and ADN gas decompose upstream of the porous media. The mole fraction distributions of nitrogenous compounds are illustrated in Fig.3(a). ADN decomposes to NH₃, HNO₃, N₂O firstly mainly through Reaction-1. Then NH₃ and HNO₃ react to generate N₂O through Reaction-3. N₂O can be transformed to N₂ by the collision with other molecules (H₂, H₂O, CO).

The oxidization of CH₃OH and the decomposition of ADN do not happen synchronously in the chamber. The decomposition of ADN happens near the inlet while the CH₃OH is oxidized downstream of the porous media. The mole fraction distributions of carbonous compounds are illustrated in Fig.3(b).

CH₃OH turns to CH₂OH, CH₂O, HCO and CO step by step through dehydrogenation reactions. Little CO is oxidized to CO₂. Some part of CH₃OH gas does not participate in the chemical reaction and is ejected out of the nozzle. The mole fractions of CH₂OH and HCO are very little because these two intermediates are in steady state which means that the consumption and regeneration of them occur at rapid but approximately equal rate.

The temperature of gas in chamber is nearly 1100K, far below the adiabatic combustion temperature (nearly 2600K). Two processes, including the evaporation of propellant and the heating process to porous media, absorb much heat release of the chemical reactions and make a non-adiabatic combustion for ADN and CH₃OH gas. The transformation from N₂O to N₂ and the oxidization of CH₃OH and are two main chemical processes of the second stage, the temperature range of which is 1400K to 2600K. These chemical processes can not be completed under the chamber temperature so that there is some N₂O and CH₃OH in the exhaust gas.

Table 1: The Chemical Reactions of ADN-CH₃OH

	Reactions	A	n	E_a
1	$\text{NH}_4\text{N}(\text{NO}_2)_2 \rightleftharpoons \text{NH}_3 + \text{N}_2\text{O} + \text{HNO}_3$	5.00×10^{13}	0.0	2000.0
3	$\text{NH}_3 + \text{HNO}_3 \rightleftharpoons \text{N}_2\text{O} + 2\text{H}_2\text{O}$	2.00×10^9	0.0	2000.0
8	$\text{N}_2\text{O} + (\text{M}) \rightleftharpoons \text{N}_2 + \text{O} + (\text{M})$ Low/ 6.37×10^{14} 0 $5.664 \times 10^{14}/$ H ₂ /2.00/ H ₂ O/6.00/ CO/1.50/	7.91×10^{10}	0.0	56020.0
16	$\text{HCO} + \text{M} \rightleftharpoons \text{H} + \text{CO} + \text{M}$ H ₂ /2.00/ H ₂ O/12.00/ CO/1.90/	4.75×10^{11}	0.7	14870.0
24	$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{HCO} + \text{H}_2$	5.74×10^7	1.9	2749.0
27	$\text{CH}_2\text{OH} + \text{M} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}$	1.00×10^{14}	0.0	25100.0
33	$2\text{CH}_2\text{OH} \rightleftharpoons \text{CH}_3\text{OH} + \text{CH}_2\text{O}$	3.00×10^{13}	0.0	0.0
35	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2$	3.20×10^{13}	0.0	6095.0
40	$\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$	2.23×10^5	1.9	-1158.7

Table 2: The comparison of numerical and experimental results

	numerical result	experimental result	deviation
P/MPa	0.45	0.48	6.2%
T_g/K	1093	1170	6.5%
x_{CO}	1.32%	1.6%	17.5%
x_{NO}	$5.16 \times 10^{-3}\%$	0	

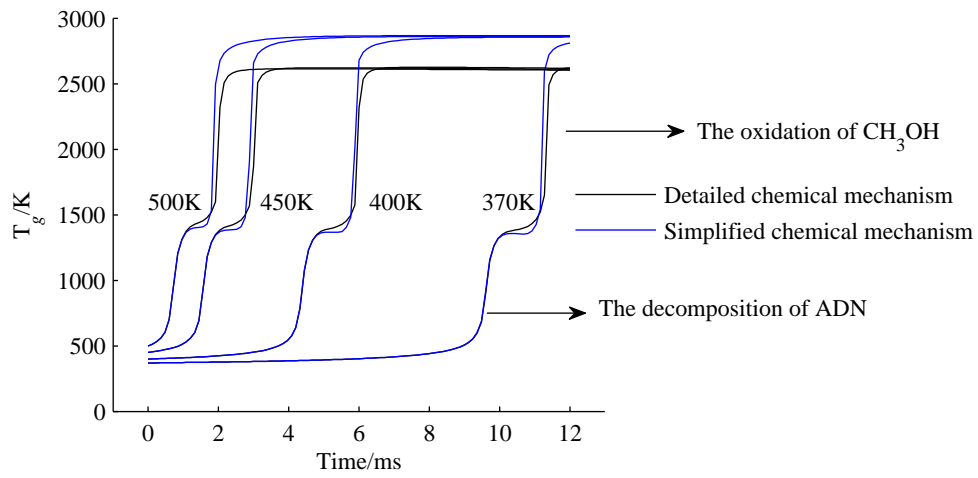


Figure 1: The ignition processes at different initial temperature

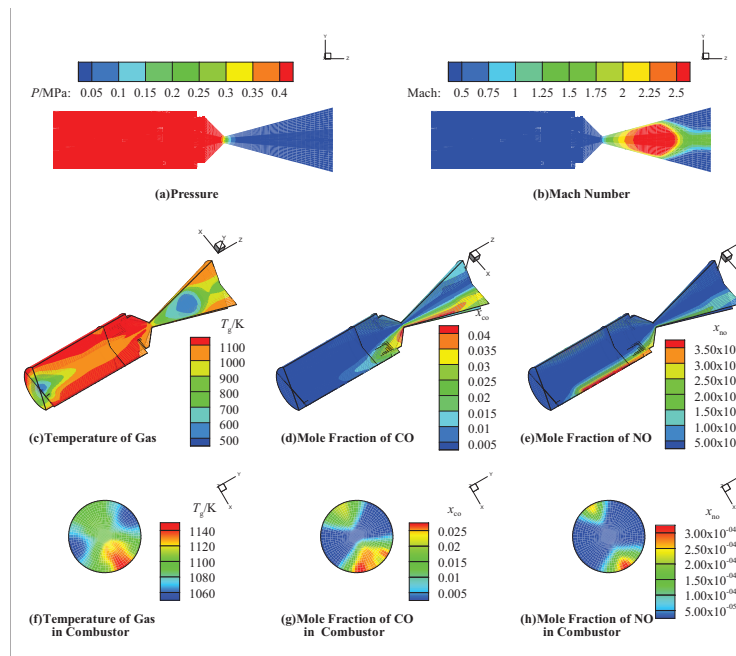


Figure 2: Some numerical results for steady operation mode

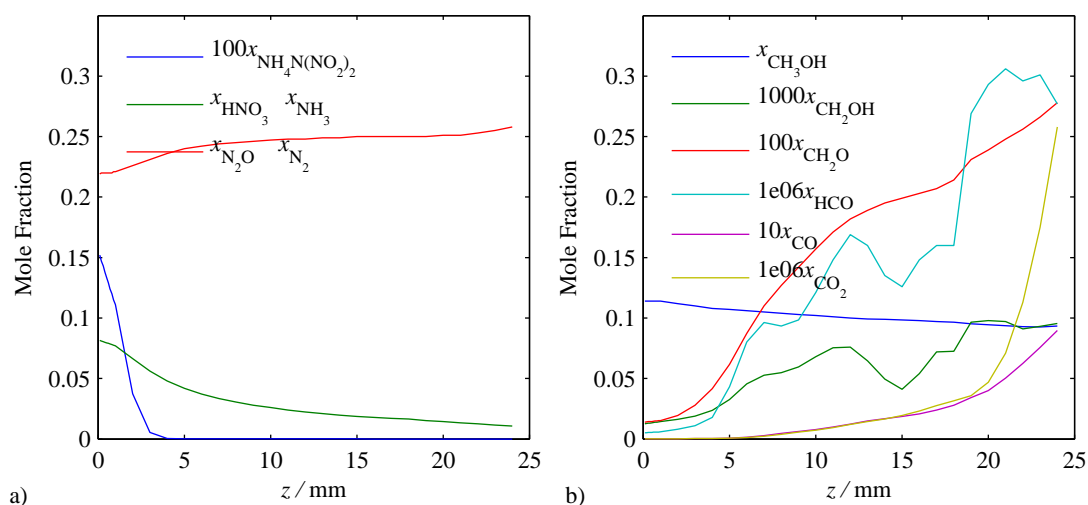


Figure 3: The numerical results of mole fraction distributions along the combustion chamber

References

- [1] Yang R, Thakre P, Yang V. (2005). Thermal decomposition and combustion of ammonium dinitramide (review). *Combustion Explosion and Shock Waves*. 41(6):657-679.
- [2] Larsson A, Wingborg N. (2011). Green Propellants Based on Ammonium Dinitramide (ADN). *Advances in Spacecraft Technologies*. 139-156.
- [3] Anflo K, Grönland TA, Wingborg N. (2000). Development and testing of ADN-based monopropellants in small rocket engines. 36th AIAA/ASME/SAE/ASEE Joint Propulsion Conference
- [4] Mujeebu MA, Abdullah MZ, Bakar MZ, Mohamad AA, Abdullah MK. (2009). A review of investigations on liquid fuel combustion in porous inert media. *Progress in Energy and Combustion Science*. 35(2):216-230.
- [5] De Reuck KM, Craven RJB. (1993). Methanol. *International Thermodynamic Tables of the Fluid State*. 12
- [6] Cheng NS, Qiao CK, Chen XW, Liu XN. (2014). Application of pseudo-fluid approximation to evaluation of flow velocity through gravel beds. *Powder Technology*. 260:15-21.
- [7] Zhiguo Z, Maozhao X. (2008). Numerical simulation about interaction between pressure swirl spray and hot porous medium. *Energy Conversion and Management*. 49(5):1047-1055.
- [8] Korobeinichev OP, Bolshova TA, Paletsky AA. (2001). Modeling the chemical reactions of ammonium dinitramide (ADN) in a flame. *Combustion and Flame*. 126(1-2):1516-1523.
- [9] Li J, Zhao Z, Kazakov A, Chaos M, Dryer FL, Scire JJ. (2007). A Comprehensive Kinetic Mechanism for CO, CH₂O, and CH₃OH Combustion. *International Journal of Chemical Kinetics*. 39:109-136.