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Numerical and experimental studies on nozzle two-phase flow characteristics of nanometer-scale iron powder metal fuel motor

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ABSTRACT

Metal iron powder is a promising new type of energy source that is of enormous practical and research interest for future automotive power systems. To better optimize engine design, this study was devoted to the characteristic investigation of a two-phase flow. Experimental studies involving nanometer iron powder particle combustion and engine thrust measurement were conducted to confirm the results obtained from numerical calculations that were performed using a fourth-order Runge–Kutta–Gill method. Governing equations for nozzle two-phase flow were established to perform a theoretical study to analyze the combustion properties of iron oxide particles and flow in the nozzle. The results indicate that variations in the size and coagulation content of particles play a significant role in the loss of two-phase flow. Significant emphasis was placed on the effect of particle size (0.4–1.0 μm) and condensate content (10–40%) of ultrafine particles on the specific impulse. To further validate the theoretical results, the burning rates of particles of three different sizes were experimentally measured. In addition, the motor thrust and the specific impulse with the particle size of 50 nm were tested through combustion experiment, and the results show excellent agreement.

1. Introduction

Recently, metal fuel (such as **Fe, Mg, Al, Li, Be,** and **B**) motors have been introduced to replace diesel–electric engines as they involve completely taking advantage of its high volumetric energy. This involves a violent reaction under certain conditions with water or oxygen that produces a significant amount of heat energy. In particular, the energy density of iron powder significantly exceeds that of fuel oil or coal, and its oxide can be readily recycled, and exhaust pollution is not generated. Thus, its numerous advantages are examined to compensate for the shortage of energy sources and for its wide application prospects in the future.

Researchers in countries including Russia, Ukraine, and the United States recently conducted a series of studies on the metal fuel engine. In particular, the technology in both Russia and Ukraine was applied to supercavitating torpedoes at advanced levels. For example, the "Snowstorm" usually employs magnesium powder as a fuel with a speed of 200 kn. The United States Applied Research Laboratory (ARL) [1,2] studied **Al/H_2O** and **Mg/H_2O** system performance with high-pressure carrier-gas mode and successfully tested the principle of an engine test.

Metal fuels, such as iron powders, are used for water transportation energy systems and are also widely used for automobile power devices or remote area workstations. Metal iron powder is one of the most promising new energy sources for the future [3–5]. However, a major difficulty in the numerical study of two-phase flow peculiarities involving the combustion of nanometer iron powder particles in an oxygenous atmosphere requires the establishment of appropriate mathematical models. Research on nozzle two-phase flow characteristics is an indispensable theoretical foundation for engine system optimization design and an important research topic. For example, Kleist [6] conducted a series of investigations with respect to gas–solid two-phase flow via computer simulations and accurately predicted the velocity of solid particles. Yeung [7] also examined the characteristics of the gas–solid two-phase flow at the entrance of a circular pipe and analyzed the dynamic flow characteristics of the particles by assuming that the fluid is incompressible and corresponds to an indiscerptible stratified fluid. Subsequently, in [8], Huh et al. indicated that the flow of micro-channel surface wettability and the spatial distribution of water to air significantly impacts the two-phase flow. In [9], the authors reported an optimal design

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Table 1
Comparison of energy performance of several types of metal fuels.

Metal fuel									Metallic oxide		
Name	Molecular weight	Density/ kg·m^{-3}	Melting point/K	Boiling point/K	Reaction with water		Reaction with oxygen		Name	Melting point/K	Boiling point/K
					Mass energy/ MJ·kg^{-1}	Volume energy/MJ·L^{-1}	Mass energy/MJ· kg^{-1}	Volume energy/MJ·L^{-1}			
Fe	55.84	7.86×10^3	1811 [29,32]	3273	0.902	7.091	7.397	58.14	**Fe_2O_3**	1839 [29,32]	–
Al	26.98	2.70×10^3	933	2767	17.61	47.54	31.054	83.847	**Al_2O_3**	2315	3250
Mg	24.30	1.74×10^3	923	1366	14.81	25.77	24.761	43.085	**MgO**	3098	3850
Li	6.94	0.53×10^3	454	1620	28.61	15.16	42.998	22.79	**Li_2O**	1843	2836
Be	9.01	1.85×10^3	1560	2744	36.03	66.67	62.700	116.00	**BeO**	2720	3580
B	10.81	2.34×10^3	2450	3931	18.81	44.02	267.06	624.94	**B_2O_3**	723	2320

for nozzle two-phase flow by conducting a **CO_2** nozzle two-phase flow experiment. Further, Ali et al. [10] examined the influence of the contraction ratio on nozzle two-phase flow combined with the mass transfer based on the Euler numerical method and improved carbonation efficiency by modifying the nozzle geometry. Furthermore, in [11], Piroozian et al. experimentally studied the flow pattern of a waxy crude oil and water in a carbon steel horizontal pipe. In [12], the author utilized a splitting strategy to simulate compressible two-phase flows and conducted several numerical simulations based on two-dimensional structured grids. Similarly, in [13], Teixeira et al. performed numerical investigations to obtain a solution for the steady-state one-dimensional drift-flux model and employed a SIMPLER semi-implicit algorithm in the solution of the finite-volume discretized model.

Metal iron powder was earlier studied in 1983 by Beach et al. [14] because of an interest in the function of iron clusters in catalytic systems and biological electron carriers. Further, Beach et al. [5,15] employed nanometer iron powder as a vehicle engine fuel. The study indicated that a 50-nm powder exhibited significantly better activity in comparison to other large particles. Although there are a few key techniques that should be further developed for the application of metal iron powder as a fuel (such as burning rate governing technology, metal particle-size optimization processing, waste collection technology, and engine fuel-delivery system design), it is still of overwhelming research interest.

Potentially, metal iron powder is a desirable alternative for automotive engine fuel. However, previous studies on metal engine fuels have mostly focused on aluminum [16–20], magnesium [2,21], or aluminum–magnesium propellant [22–24], There has been a lack of research on the iron powder motor, and research has been limited to the stage of combustible characteristic analysis [25–30]. For example, Wen et al. [31] performed an experimental study on the heating and oxidation of iron nanoparticles in a simultaneous TGA/DSC system. The results demonstrate that heat release recorded by DSC is in the range of 1.67–2.92 kJg^{-1}, and the activation energy of iron nanoparticles ranges within 0.9–1.9 eV with decreasing heating rates. Moreover, in [30] an in-depth analysis of the iron-to-FeO oxidation reaction in the context of laser–oxygen cutting of mild steel was presented. In [32], the combustion characteristics of nanofluid fuels containing boron (~80 nm) and iron particles (~25 nm) were investigated, and it was found that some of the iron particles were burned simultaneously with the liquid droplet, and the rest formed a large agglomerate on fiber at a later stage. Recently, Julien et al. [33] experimentally examined the flame structure of methane–iron–air flames for particles reacting in diffusion-controlled or kinetically-controlled regimes using various oxidizing mixtures. Similarly, in a study by Schiemann et al. [34], a numerical model for iron particle combustion was developed and implemented in a commercial computational fluid dynamics (CFD) solver, and the standard geometry of an industrial-scale spray roaster was chosen to substitute a gaseous fossil fuel partially by iron particles.

Although nanometer iron powder shows excellent energy density, reaction activity, and combustion performance, and it is a pollution-free engine fuel, studies on its nozzle two-phase flow properties are lacking. There is room for considerable research in this field. The calculation results in Table 1 indicate that the volume energy in iron powder reacts with oxygen and reaches up to 58.14 MJ/L, as indicated by the calculation of chemical reaction standard molar enthalpy [35]. In comparison, beryllium possesses the highest calorific power of 36.03 MJ·kg^{-1} in hydro-reactive metal fuel. However, it is not suitable for applications because of the toxicity of its combustion products. Boron is invariably employed as a torpedo propellant due to its high-energy density or excellent performance, but it can only be applied in military projects as it is extremely expensive. It is not difficult for either magnesium or lithium to react with water, although it is low in volume energy. Although aluminum presents more advantages (such as high reaction caloric, stability, and non-toxicity), in comparison to other metals, the product of **Al_2O_3** prevents a sustaining reaction due to its tough shell. Moreover, surface treatment technology is a major problem. Comparatively, iron is most suitable for automobile fuel because of its numerous advantages, and the calorific intensity of combustion reaches up to 7397 KJ/kg with a particle size of 50 nm. Hence, nanometer iron powder is a preferred substitute for fuel oil.

In this study, we performed several investigations on the two-phase flow property in an iron powder metal fuel motor. We studied the behavior of particle combustion and the effects of particle size and condensed phase content on the specific impulse through numerical computation and experimental validation. It is expected that the analysis results of the study will help in further optimizing engine design and improving motor performance.

2. Experiment

The design of the experiment on the metal fuel engine is summarized as follows. (1) The engine system was mainly composed of an ignition device, a combustion chamber (external dimension: ϕ50 mm × 300 mm, internal diameter: ϕ30 mm), a nozzle, an intake valve, a temperature sensor, and a pressure sensor. (2) The fuel was mainly composed of nanometer iron powder (50-nm particles were coated with a thin layer of carbon about 2–3 nm thick to prevent oxidation), oxidizer ammonium perchlorate (AP), and other ingredients, including a binder (HTPB), a catalyst (copper oxide), and other substances in a certain proportion (the metal iron powder column with a size of ϕ25 mm × 150 mm prepared by special preparation process was employed as a propellant). (3) The ignition device consisted of ignition powder and a 12-V power supply for ensuring effective ignition. (4) Both the temperature and pressure sensors served as real-time data technologies for measuring the combustion chamber pressure and temperature. In addition, the pressure was maintained at 5 MPa throughout the experiment to ensure sustained and stable combustion of the iron

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