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Short communication

Effect of aluminum nanoparticles on combustion characteristics and pollutants emission of liquid fuels – A numerical study

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ABSTRACT

The combustion characteristics and pollutants emission of ethanol and *n*-decane liquid fuels with the addition of aluminum nanoparticles have been numerically investigated. The results reveal that Al nanoparticles lead to a reduction of flame temperature of ethanol and decane fuels. Also the temperature peak location will be shifted toward downstream. In addition, mass fraction of pollutants CO and NO_x will be decreased by adding nano-aluminum to these fuels. These findings confirm that aluminum nanoparticles improve combustion features of ethanol and decane fuels.

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1. Introduction

Nanofluids, solutions containing a stable suspension of nanoparticles (e.g., metals, oxides, carbides, nitrides, or carbon nanotubes) with typical lengths of 1–100 nm, have attracted great interest recently [1–7]. Because of their enhanced thermal conductivity, nanofluids can be used in energy-related systems. Murshed et al. [8] provided a comprehensive review of nanofluids applications in transportation, micromechanics and instrumentation, heating, ventilating and air-conditioning (HVAC) and medical fields.

Because of high surface area, nanoscale energetic materials offer high reactivity, shortened ignition delays and fast energy release [9]. According to Jackson et al. [10], addition of aluminum nanoparticles could substantially decrease the ignition delay time of slurries of *n*-dodecane. Tyagi et al. [11] by using a simple hot-plate experiment, found that nano-aluminum significantly enhance the ignition probability of diesel fuel. Beloni et al. [12] studied effects of pure aluminum, mechanically alloyed Al_{0.7}Li_{0.3} and nanocomposite 2B + Ti as nano additives on flame length, flame speed and flame temperature of decane-based slurries. Comparing the burning characteristics of fuel droplets with nano- and micron-sized aluminum particles, Gan and Qiao [13] showed that for the same solid loading rate and the same surfactant concentration, the microexplosion behavior of the micron suspension occurred later than the nanosuspension with much stronger intensity. Solero [14] results revealed that addition of Al₂O₃ nanoparticles to diesel fuel can improve the combustion features of the spray flame and giving rise to lower CO emission levels.

These previous studies have revealed some ignition characteristics of fuels with the addition of nanoparticles. However the effect of nanoparticles on combustion characteristics and pollutants emission of fuels has been rarely investigated. The objective of this paper is to numerically determine the combustion features of ethanol and *n*-decane liquid fuels with the addition of Al nanoparticles.

2. Description of physical model

The flow configuration investigated in this paper is based on a non-premixed swirl-burner. Liquid fuel droplets are injected from the center of a combustion chamber while hot air stream flows around them. The flow has been considered to be two-dimensional and axi-symmetric. Air flow temperature is higher than boiling-point temperature of liquid fuel which causes quick evaporation of droplets. The Re number is around 100, the swirl number is set to 0.25 and air inlet axial velocity is 6 m/s. In Fig. 1, the computational domain and the employed boundary conditions are shown together. In order to check grid independency of the results, three grid meshes were tested. Fig. 2 presents the temporal evolution of droplet mass obtained by employing these grid meshes. From this figure, it is reasonable to select 100×36 grid nodes as a good compromise between accuracy and computational time.





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$\begin{array}{ccc} C_p & \text{constant-pressure specific heat (J/kg K)} & \rho & \text{density (kg/m^3)} \\ D & \text{droplet diameter (m)} & & \\ M & \text{molecular weight (g)} & & Subscripts \\ S & \text{source term} & nf & \text{nanofluid} \\ t & \text{time (s)} & 0 & \text{initial} \\ u_i & \text{velocity component (m/s)} & s & \text{nanoparticle} \\ \hline \\ $	Nome	nclature		
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Φ diffusion parameter	${oldsymbol{\Phi}}$	diffusion parameter		

3. Mathematical model

The governing equations for the gas phase are Reynolds-Averaged Navier–Stokes, energy and species concentration. Turbulence stresses in gas phase equations are modeled by k- ϵ method, so two transport equations are also required for turbulent kinetic energy and eddy dissipation rate. The set of governing equations can be conveniently written in a general transport equation form as follows [15]:

$$\frac{\partial}{\partial t}(\rho\Phi) + di\nu(\rho u_i\Phi) = di\nu\{\Gamma_{\Phi} \ grad\Phi\} + S_{\Phi}$$
(1)

This generalized transport equation contains transient, convection, diffusion and source terms, respectively where the general variable Φ may represent the mean value of any unknown variable in the aforementioned governing equations. The parameters Γ_{Φ} and S_{Φ} represent an effective diffusion coefficient of this general variable and the source term respectively. It has to be noted that in the near-wall region, a wall-function approach is used to bridge the viscous sublayer. The gas phase governing equations are solved using SPRINT code [16] which has been validated before against experimental data.

The time-dependent Lagrangian momentum equations for liquid phase are solved numerically to determine velocity and position of droplets [17,18]. The mass conservation equation for liquid phase is obtained using correction factor introduced by Nicos and Dean [19]. Also by using the correlation reported by Faeth [20] the heat transfer equation is obtained. Clausius–Clapeyron equation of state [21] is employed to predict phase behaviors of system.

The effect of nanoparticles on liquid phase equations is modeled by revising the thermo-physical properties according to following equations [22,23] for density, molar mass and heat capacity.

$$\rho_{nf} = (1 - \phi)\rho + \phi\rho_s \tag{2}$$

$$M_{nf} = (1 - \phi)M + \phi M_s \tag{3}$$

$$(\rho C_p)_{nf} = (1 - \phi)\rho C_p + \phi \rho_s C_{\rho,s} \tag{4}$$

where properties with subscript "s" are for nanoparticles while without subscripts are for basefluid. The variable ϕ in above equations represents nanoparticles volume fraction.

Influence of Al nanoparticles on understudied fuels heat of vaporization is obtained using published experimental data of Gan and Qiao [24]. From their results, the difference between the evaporation rate of nanofluid and its base fluid could be obtained and then by employing the well known D²-law, nanofluid enthalpy of vaporization can be calculated.

For mathematical modeling of combustion phenomenon, twostep Magnussen model has been used and hence for each chemical species, one transport equation must be solved. In addition, Zeldovich model has been employed to model thermal NO_x emission in the system.



Fig. 2. Temporal evolution of droplet mass for three computational grid meshes.



Fig. 1. Computational domain and employed boundary conditions.

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