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Study on combustion characteristics of dimethyl ether under the moderate or intense low-oxygen dilution condition

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ABSTRACT

Experiments and numerical simulations were conducted in this paper to study the combustion behavior of dimethyl ether in the moderate or intense low-oxygen dilution regime, in terms of thermal/chemical structure and chemical kinetics associated with nitrogen oxide and carbon monoxide emissions. Several co-flow temperatures and oxygen concentrations were involved in the experiments to investigate their impacts on the flame behavior systematically. The results show that in the moderate or intense low-oxygen dilution regime, oxygen concentrations in the flame base slightly increased because of the prolonged ignition delay time of the reactant mixture due to oxidizer dilution, which changed the local combustion process and composition considerably. The oxidation rates of hydrocarbons were significantly depressed in the moderate or intense low-oxygen dilution regime, such that a fraction of unburned hydrocarbons at the furnace outlet were recirculated into the outer annulus of the furnace, which changed the local radial profiles of carbon monoxide, methane, and hydrogen partially. Moreover, with the increment in co-flow temperature or oxygen mole fraction, flame temperature, and hydroxyl radical, carbon monoxide, and hydrogen mole fractions across the reaction zone increased gradually. For the dimethyl ether-moderate or intense low-oxygen dilution flame, temperature homogeneity was improved at higher co-flow temperature or lower oxygen mole fraction. The carbon monoxide emission depended on the levels of temperature and hydroxyl radical concentration inside the reaction zone significantly. Emission index of carbon monoxide increased at lower co-flow temperature or oxygen mole fraction; and it was more sensitive to the variation in co-flow oxygen mole fraction. Additionally, the dominant formation pathways of nitrogen oxide in the dimethyl ether-moderate or intense low-oxygen dilution flame were clarified. The contribution of the thermal pathway was fairly unimportant. Emission index of nitrogen oxide increased as co-flow temperature or oxygen mole fraction was increased. The ratio of nitrogen dioxide emission index to nitrogen oxide emission index decreased with the increment in co-flow temperature or oxygen mole fraction.

1. Introduction

Dimethyl ether (DME, CH_3OCH_3) is one of the most promising alternative fuels emerging in the past few decades. By comparing its properties with those of the traditional fuels, Arcoumanis et al. [1] concluded that DME had the potential of substituting for the liquefied petroleum gas (LPG), diesel fuel, and liquefied natural gas (LNG).

DME can be produced from a variety of traditional energy sources in large amounts, such as coal, natural gas, and biomass. The current plans in China, Sweden, Japan, and Korea to produce DME for fuel usage are a sign that DME is converting from being a fuel of the future to being a fuel of the present, as discussed in [2].

At present, DME is mainly applied to engines as a neat fuel or additive. Studies indicated that DME was a more suitable fuel for

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Nomenclature

Abbreviations

CFD	computational fluid dynamics
CI	compression ignition
DME	dimethyl ether, CH_3OCH_3
DO	discrete ordinate
EDC	eddy dissipation concept
FLOX	flameless oxidation
HC	unburned hydrocarbon
LNG	liquefied natural gas
LPG	liquefied petroleum gas
MILD	moderate or intense low-oxygen dilution
WSGGM	weighted sum of gray gas model

Latin symbols

A_i	pre-exponential factor for the *i*th reaction, its unit depends on reaction
E_{ai}	activation energy for the *i*th reaction (cal/mol)
EI_i	emission index of the *i*th species (g/kg(fuel))
k	turbulent kinetic energy of the fluids (J/kg)
L_R	length of reaction zone (mm)
l	number of oxygen atoms in the molecular structure of the species $C_mH_nO_l$, dimensionless
m	number of carbon atoms in the molecular structure of the species $C_mH_nO_l$, dimensionless
$\dot{m}_f$	mass flow rate of fuel (kg/s)
$\dot{m}^*_{O_2}$	mass flow rate of O_2 in the co-flow (kg/s)
N	total number of species in the system, dimensionless
n	number of hydrogen atoms in the molecular structure of the species $C_mH_nO_l$, dimensionless
n_C	number of carbon atoms in the molecular structure of the fuel, dimensionless
R	the universal gas constant, 1.986 cal/(mol K) (or 8.314 J/(mol K))
Re_{co}	Reynolds number of the co-flow, dimensionless
Re_f	Reynolds number of the fuel, dimensionless
r	radius of the system (mm)
T	temperature (K)
$\dot{T}^*_{CO}$	co-flow temperature (K)
T_f	fuel temperature (K)
u_{co}	co-flow velocity (m/s)
u_f	fuel jet velocity (m/s)
W_i, MW_i	molecular weight of the *i*th species (kg/mol)
X^*_i	mole fraction of the *i*th species in the co-flow, dimensionless
x, y, z	coordinates of the cartesian system, mm
Y_i	mass fraction of the *i*th species, dimensionless

Greek symbols

β_i	temperature exponent for the *i*th reaction, dimensionless
χ_{CO}	mole fraction of CO in the flue gas, dimensionless
χ_{CO_2}	mole fraction of CO_2 in the flue gas, dimensionless
χ_i	mole fraction of pollutant species *i* in the flue gas, dimensionless
ε	dissipation rate of the turbulent kinetic energy (m^2/s^3)
Φ_{global}	the global equivalence ratio inside the furnace, dimensionless
Φ_{local}	the local equivalence ratio, dimensionless

Superscript

$*$	co-flow

Subscript

f	fuel
co	co-flow

compression ignition (CI) engines versus the diesel oil. Park et al. [3] reviewed the applicability of DME in the CI engine. The clean performance of DME in the CI engine was also reviewed in [4]. Song et al. [5] studied the performance of a controllable premixed combustion engine fueled by DME, in which ultra-low NO_x emission and smoke-free operation were realized. Ji et al. [6] reported that the addition of DME to spark-ignited ethanol engine could increase the engine thermal efficiency by over 20%, and shorten the flame development and propagation duration evidently. Meanwhile, the unburned hydrocarbon (HC) emission was also reduced by DME addition, proving the potential of DME addition to improve the performance of spark-ignited ethanol engine. Additionally, Liang et al. [7] reported that HC emission of the DME-enriched ethanol engine at DME volume fraction of 2% could be reduced by 45%, in comparison with the pure ethanol case; but NO_x emission was slightly increased. Wang et al. [8] studied the combustion and emission characteristics of a diesel engine with DME as port premixing fuel under different injection timing. The heat release process and clean performance of the engine at different DME quantities were analyzed. Park et al. [9] studied the in-cylinder spray behavior of DME, as well as its effect on NO_x, CO, and HC emission characteristics in a high-speed engine. Reduction in pollutant emission of DME was reported.

More recently, DME was also introduced into the fields of industrial boiler, gas turbine, and fuel cell.

In our previous studies, Ref. [10] studied the NO_x and CO emission mechanisms of DME/air jet diffusion flame using the chemical reactor network analysis method. Ref. [11] proposed a series of empirical correlations and methods for predicting the radiative heat flux outside the DME jet diffusion flame. Ref. [12] experimentally and numerically investigated the flame structure and reaction zone size of DME/air premixed flame in an industrial boiler furnace; and the NO_x and CO emission behaviors of the DME/air premixed flame in this boiler furnace were analyzed in Ref. [13]. The flow, mixing, and combustion characteristics of DME jet diffusion flame were compared with those of methane and LPG in Ref. [14]. New correlations for predicting the length, width, and volume of these three kinds of fuel flames were developed. Ref. [15] studied the effect of H_2 addition on the comprehensive combustion characteristics of DME jet diffusion flame, in terms of flame structure, reaction zone size, air entrainment, and NO_x and CO emission indices.

Lee et al. [16] conducted experiments on an industrial gas turbine to compare the combustion characteristics of DME and methane, and reported that DME was a very clean and efficient fuel for gas turbines. Lee et al. [17] also developed a design method for the gas turbine fuel nozzle to guarantee operational reliability and low pollutant emission of the DME-fueled gas turbine.

Additionally, Seo et al. [18] studied the effect of DME addition on the performance characteristics of a direct methanol fuel cell. It was reported that the performance of DME-methanol-fueled fuel cell was improved, in comparison with those fueled by methanol only.

Jiang et al. [19] reported that the stable DME/air premixed flame at lean combustion situation could be feasibly obtained on