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Full Length Article

Numerical investigation towards HiTAC conditions in laboratory-scale ethanol spray combustion

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ABSTRACT

In the past 25 years high temperature air combustion (HiTAC) technology has been proved and utilized in industry as a promising way to increase thermal efficiency, create a relatively uniform temperature distribution, and reduce emissions of harmful pollutants such as NO_X and CO. However, due to the complexity of fuel-oil combustion, to date HiTAC is mainly applied to gaseous fuel or coal, and little is known about spray combustion under HiTAC condition. In the present study, we numerically investigate the Delft Spray-in-Hot-Coflow (DSHC) using ethanol in high temperature diluted combustion air, and extend it to more co-flow conditions. We employ different temperatures and oxygen concentrations of the co-flow in order to dilute the oxidizer/fuel before it reacts with the fuel/ oxidizer. The pressure-swirl atomizer model with an Eulerian-Lagrangian approach was implemented for the spray modeling. Collision, coalescence, secondary breakup and evaporation of the drops were taken into account. The steady laminar flamelet model for the combustion of ethanol, the Discrete Ordinate model for radiation and the k-ε model for the turbulence with enhanced wall treatment were validated by the simulation of the NIST flame under conventional conditions and then used in the current study.

The results indicate that the decreased peak temperature in many HiTAC applications with high temperature combustion air is mainly due to the reduced oxygen concentration by entraining flue gas.

In the present study, a low oxygen concentration slows the evaporation process of droplets. It results in an enlarged combustion zone, a lowered peak temperature and minor NO_X emission. However, decreasing the oxygen concentration may lead to problems of cracking, soot formation and flame extinction, especially for heavy oils. The optimization needs to be carried out based on the analysis of a specific fuel in order to create a HiTAC-like condition.

Based on the results of the current study, the 1500 K and 6%vol oxygen concentration case is considered as a HiTAC condition.

1. Introduction

High temperature air combustion (HTAC) is a promising technology for energy saving, flame stability enhancement and reduction of NO_X emission. It has been applied in many experimental and industrial applications, and also developed and reported as “moderate or intense low oxygen dilution (mild) combustion”, “flameless oxidation”, or “colorless distributed combustion (CDC)” [1–8]. In such a combustion regime, oxygen/fuel stream is diluted by a substantial amount of hot inert flue gases before it reacts with the fuel/oxygen. This results in more uniform temperature distribution and lower NO_X emission than in case of conventional combustion. To date most of the applications of HiTAC are for gaseous fuels [3–5] or solid fuels [9,10], but little is known about spray combustion under HiTAC condition [1,11]. H. Tsuji et al. [1] introduced the historical background of HiTAC technology, and described its development and practical application to different kinds of furnaces of importance in industry. Besides the gaseous and solid fuels, they investigated experimentally kerosene spray flames and reported qualitatively with photographs the states of spray flame combustion in the high temperature preheated diluted air (523 K to 1373 K), when the O_2 concentration is changed (13% to 3%), Although it was concluded that NO_X emissions reduce in the same manner as gaseous fuel, cases when the O_2 concentration in highly preheated air is lower than 15% were not further discussed. Moreover, the experimental results from NKK Keihin using heavy oil A did not show a clear trend [1]. That can be explained by the complexity of spray combustion and many unclear fundamental aspects involved in spray combustion, in particular turbulent spray combustion. Modeling of turbulent spray combustion

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however, although challenging provides a better understanding of various phenomena in the processes involved. In a real turbulent spray flame, dispersion, continuous phase turbulence modification, dispersed phase inter-particle collisions, evaporation, mixing and combustion occur simultaneously. Dealing with all these complexities and their interactions poses a tremendous modeling task [11]. Jenny et al. [11] reviewed the modeling developments of turbulent spray combustion, together with the relevant experiments of spray flame configurations presented in a structured way, with the intention to provide a database for model validation and a guideline for future investigations. The ethanol spray flame modeling presented in the current study is one of the investigations using the Delft Spray-in-Hot-Coflow (DSHC) burner.

To address all the relevant phenomena, we employ a combination of models, such as models for turbulence, atomization, secondary break-up, collision and coalescence, evaporation, radiative heat transfer, combustion, etc. These models have been validated already by the simulation of the NIST flame using methanol under conventional condition [12] and then were applied for comparison with preliminary results from the ethanol spray-in-hot-co-flow [13]. The predicted mean velocity components of the gaseous flow and the droplets, the droplet number density, and the Sauter mean diameter (SMD) of the droplets at various heights showed good agreement with the experimental data. The method to set inlet boundary conditions for the spray has been discussed and compared with direct application of data regarding measured droplet size and velocity distribution. In the application for modeling the ethanol spray-in-hot-co-flow case, relatively good agreement with experimental data of mean droplet velocity components and size distribution at various elevations has been observed, as well. It was recommended that under hot co-flow conditions, the evaporation model and the auto-ignition and local extinction processes require more efforts in order to obtain more accurate prediction in the high strain region, which is in the vicinity of the injector exit. Ma et al. [14,15] further exploited more directly all available measured data and used a “conditional droplet injection model”, in which large droplets are injected within a small range of angle around the main spary trajectory while small droplets are injected in a much wider range. In this way the prediction of SMD in low droplet number density region also showed good agreement with the experimental data, as well as in the vicinity of the injector exit.

However, with the DSHC setup, the co-flow temperature and oxygen dilution cannot be varied independently [16]. As a result, the temperature, velocity of gas and liquid, gas components in the co-flow and their distribution vary depending on the investigated test case. Furthermore, due to the performance of the atomizer under different co-flow temperature conditions, the mass flow of ethanol can be different from the designed one. This can be verified by the reported injection pressure and mass flow rate of ethanol [17]. As a result, in order to investigate the influential parameters on combustion characteristics, we focus on a comparative numerical study of cases with different co-flow temperatures and O_2 concentrations using the validated models in a wider range than studied experimentally.

In the present research, we used different co-flow temperatures (300 K, 600 K, 900 K, 1200 K and 1500 K) and oxygen concentrations (21%, 18%, 15%, 12%, 9% and 6%) of the co-flow. The mass flow rate and pressure of the fuel-oil are kept constant. The simulation results from different cases, such as temperatures, flame profiles, droplet size distributions, etc., are studied with respect to HiTAC conditions.

As we discussed in [12], both the boundary condition and spray trajectory analysis are essential for validation of spray flames. The validation of the DSHC ethanol spray flame requires both a well-defined boundary condition of co-flow and a detailed analysis of spray trajectory. To clearly identify the influence of temperature and oxygen concentration in the coflow we here study two typical operation conditions of DSHC test rig, i.e. cold co-flow condition (300 K, 21% vol O_2) and hot co-flow condition (1500 K, 6% vol O_2), keeping the composition of the rest of the coflow identical. They represent spray flames under conventional condition and towards-HiTAC condition, respectively.

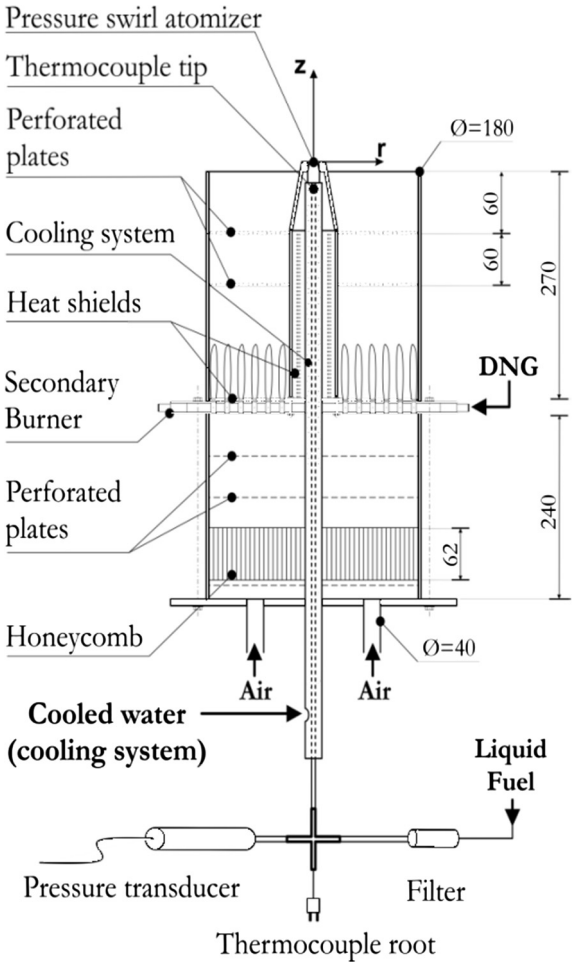

Fig. 1. Schematic of the Delft spray flame set-up (mm).

2. Numerical cases

The numerical cases are based on the experimental set up available at Delft University of Technology using the DSHC burner. Fig. 1 presents a schematic of the Delft spray burner [17,18]. An ethanol spray is produced by a pressure swirl atomizer, whereas the hot co-flow is assured by secondary burner whereby air and Dutch natural gas (DNG) mix and generate a matrix of 236 lean flames. The air/DNG ratios in combination with the effects of two perforated plates located along the pipe length dictate the temperature, oxygen and turbulence levels. Co-flow composition and temperature are selected to emulate the conditions of flue gas in large scale furnaces. This design enables a wide range of co-flow characteristics with good axisymmetric properties without the need for elaborate safety systems and allows easy optical access to laser diagnostics.

3. Mathematical models

The mathematical formulation for turbulent spray combustion simulation consists of the consideration of the computational grid, turbulence model, spray model, radiation and combustion model, NO_X model etc. Since these models and methods are expected to be validated and developed to generate the knowledge needed for the extension of the application of HiTAC technology to other fuel oils in various applications, for which detailed reaction mechanisms may still need to be investigated and various geometries of chambers/furnaces may be involved, the Reynolds averaged equations are employed, using ANSYS Fluent software. As a result, the models used in the study remain as general as possible in order to be implemented for various applications.