

# The Structure of Nonpremixed Ethanol Flames

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## Abstract

An experimental and kinetic modeling study is carried out to elucidate key aspects of non-premixed combustion of ethanol. The experimental studies are performed on flames stabilized in the coflow configuration. In this configuration two reactant streams flow parallel to each other. The reactant streams are introduced into a mixing layer above two concentric segments: an inner segment and an outer segment. Fuel stream made up of a heated mixture of prevaporized ethanol and nitrogen is introduced from the inner segment into the mixing layer. Preheated air stream is introduced from the outer segment. Measurements made include flame structure and critical conditions of blow-off. The flame structure is measured by removing gas samples from the flame and analyzing the samples using a gas chromatograph. Temperature profiles are measured using coated thermocouples. Critical conditions of blow-off give the mass fraction of ethanol in the fuel stream as a function of the velocity of the fuel stream at blow-off. Kinetic modeling of the experimental data is performed using the San Diego Mechanism. The numerical simulations are carried out using the commercial CFD software FLUENT 6.3. Flame shapes, flame structure and critical conditions of blow-off are calculated and compared with experimental data.

## 1 Introduction

Alcohols, in particular, ethanol ( $C_2H_5OH$ ) are frequently mentioned as alternative fuels. They can be produced in large quantities from agricultural products such as corn, wheat, sugar-cane, and wood, or from waste products such as sewage and municipal waste. Alcohols are renewable fuels because they can be produced from biomass fermentation and are by-products of Fischer Tropsch processes. Ethanol is currently a component of reformulated gasoline. The amount of ethanol in gasoline is projected to increase in the future. Numerous studies have addressed premixed and nonpremixed combustion of ethanol [1, 2, 3, 4, 5, 6, 7, 8, 9]. Studies on premixed combustion include measurements of burning velocities and extinction strain rates. Studies on nonpremixed combustion were focused on flames stabilized in the counterflow configuration [5, 8]. In these studies critical conditions of extinction were measured and compared with predictions of kinetic models. The present study is on nonpremixed combustion of ethanol stabilized in the co-flow configuration. Here the flame structure and critical conditions for blow-off are measured and compared with predictions of kinetic models.

## 2 Description of the Experimental Apparatus

The components of the experimental apparatus are (1) the co-flow burner assembly, (2) the gas handling system, (3) the vaporizer and liquid fuel handling system, and (4) heating and temperature control system.

Figure 1 shows a schematic illustration of the burner assembly. The reactant streams are introduced into

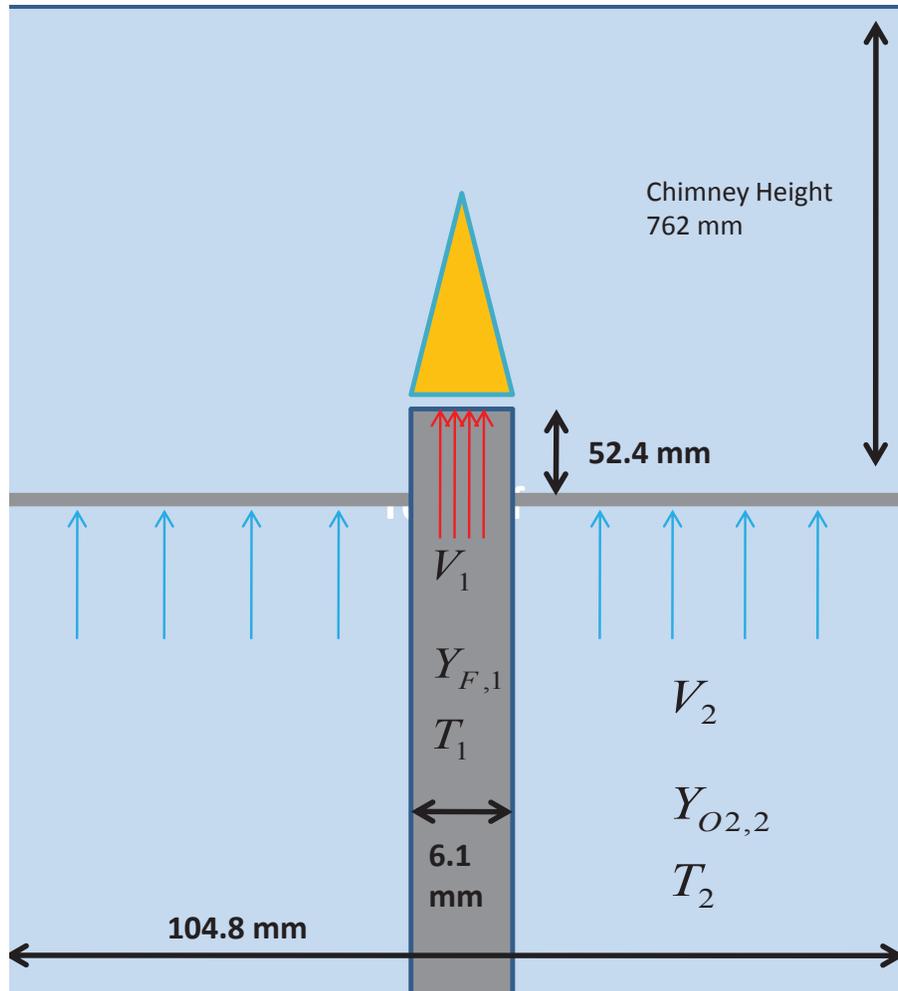


Figure 1: Schematic illustration of the coflow burner.

a mixing layer above two concentric segments: an inner segment and an outer segment. Fuel stream made up of a heated mixture of prevaporized ethanol and nitrogen is introduced from the inner segment into the mixing layer. Preheated air stream is introduced from the outer segment. The inner segment is made of stainless steel tubes. It has an exit diameter of 6.1 mm. The mass fraction of fuel, the temperature and the injection velocity at the exit of the inner segment are represented by  $Y_{F,1}$ ,  $T_1$ , and  $V_1$  respectively. The outer segment is made of aluminum. The inner diameter of the outer segment at the exit is 104.8 mm. The exit of the outer segment is about 52.4 mm below the exit of the inner segment. A quartz chimney is mounted at the exit of the outer segment. Several layers of inconel screens are placed in the outer segment to make the flow parallel. As a consequence plug-flow boundary conditions can be used. Heating tape is wrapped around the outer segment to prevent condensation. The temperature and

flow velocity at the exit of the outer segment is represented by  $T_2$ , and  $V_2$  respectively. Thermocouples are placed near the entrance where the heated reactants enter into the coflow burner to record the temperature.

The gas handling system is comprised of air, and nitrogen that is mixed with the fuel. A syringe pump is used to introduce liquid fuel into a Sono-Tek Accumist nozzle. Nitrogen is introduced into the nozzle. The flow rate of nitrogen is accurately measured using a mass flow controller. A mixture of fuel mist, with a mean size of 15 microns, and nitrogen is produced. The mist enters a heated vaporizer where the fuel is completely vaporized. The heated mixture of nitrogen and prevaporized fuel is introduced into the co-flow burner. The mass flow rate of the co-flow air is measured using a mass flow meter. It is heated and introduced into the coflow burner. To prevent condensation of the prevaporized fuel, the air line to the coflow burner, the vaporizer, and the fuel line from the vaporizer to the coflow burner are heated with three separate heating tapes. The temperatures of these lines are maintained at selected values using three separate PID temperature controllers coupled to individual solid state relays. Each temperature controller analyzes data from the three K-type thermocouples mounted in the vaporizer, air line, and fuel line. The controllers adjust the duty cycle of the electric current supplied to each group of heating tapes such that the temperature in each line is maintained at the selected value. The controllers maintain the temperatures of the flow lines at values high enough to prevent condensation in the lines, and low enough to prevent thermal breakdown of the prevaporized fuel. Excellent temperature control was achieved, with the temperature variation being less than  $\pm 2$  K. To make sure that there was no condensation of fuel, a steady flame was stabilized in the burner. The fuel supply was abruptly shut off. This caused the flame to extinguish immediately. If there was condensation of fuel in the lines, the flame would not have extinguished immediately. This test confirmed that there was practically no condensation of fuel in the flow lines.

The mass flow rate of the fuel is estimated from the measured volumetric flow rate of fuel obtained from the syringe pump. The mass fraction of fuel  $Y_{F,1}$  is estimated from the measured mass flow rate of nitrogen obtained from the mass flow controller and the mass flow rate of fuel. The velocity of the mixture of prevaporized fuel and nitrogen at the exit of the inner segment,  $V_1$ , and the velocity of preheated air at the exit of the outer segment  $V_2$ , are estimated from their respective measured volumetric flow rates and cross sectional area of the segments.

Experiments are carried out with ethanol as the fuel. Figure 2 shows a photograph of a flame stabilized in the coflow burner. The flame was steady with very little fluctuation. Critical conditions of blow-off are measured giving the values of  $V_1$  as a function of  $Y_{F,1}$  at fixed values of  $V_2$ ,  $T_1$ , and  $T_2$ . For  $T_1 = T_2 = 423$  K, and  $V_2 = 0.419$  m/s, blow-off is observed at  $Y_{F,1} = 0.278$ , and  $V_1 = 0.88$  m/s. The flame structure giving profiles of stable species are measured using a gas-chromatograph. Temperature profiles are measured using coated thermocouples.

### 3 Description of the Numerical Model

Kinetic modeling of the experimental data is performed using the San Diego Mechanism [10, 11, 12]. This mechanism along with the thermodynamic and transport data can be downloaded from the web [12]. The numerical simulations are carried out using the commercial CFD software FLUENT 6.3 [13]. The salient features of the numerical combustion model include optically thin approximation based thermal radiation sub-model. Appropriate model parameters available in FLUENT have been chosen and user defined functions (UDF) have been included wherever required. The effect of normal gravity has also



Figure 2: Photograph of a coflow flame. The fuel stream is a mixture of prevaporized ethanol mixed with nitrogen, with  $Y_{F,1} = 0.4$ ,  $V_1 = 0.579$  m/s and  $T_1 = 423$  K. The oxidizer stream is air with  $V_2 = 0.419$  m/s, and  $T_2 = 480$  K,

been included in the model. A finite volume method based approach along with suitable upwind scheme for convection terms and SIMPLE type algorithm for velocity-pressure coupling, is employed for discretizing the governing transport equations. Appropriate solution techniques have been employed for solving the discretized equations. Transport of any species in the mixture is modeled using the Fick's law of diffusion. Thermophysical properties of the species have been calculated as functions of temperature and species concentrations. The properties of each species as a function of temperature have been calculated using kinetic theory and CHEMKIN thermodynamic database. Viscosity, binary mass diffusivity and thermal conductivity are calculated using kinetic theory. Further details of the numerical formulation are given elsewhere [14].

The boundary condition are identical to those in the experiment. Flame shapes, flame structure and critical conditions of blow-off are calculated and compared with experimental data.

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