the ENERGY lab

PROJECT FACTS

Hydrogen Turbines

Turbulent Flame Speeds and NO_x Kinetics of High Hydrogen Content Fuels with Contaminants and High Dilution Levels—Texas A&M University

Background

Turbine design in power systems utilizing high hydrogen content (HHC) synthesis gas (syngas) fuel is impacted by flame speeds, ignition behavior, and nitrogen oxide (NO_x) emissions. The main components of this fuel are hydrogen (H_2) and carbon monoxide (CO), but the variability of the source and the synthesis process can result in a wide range of possible fuel blends that can also contain carbon dioxide (CO_2), water (H_2O), and impurities. In this project, Texas A&M University (TAMU) will add to the data already accumulated on the properties and fuel reactivity of syngas combustion in turbines and offer a validated chemical kinetics model that can be utilized for the design of new turbine power systems.

This project was competitively selected under the University Turbine Systems Research (UTSR) Program that permits academic research as well as student fellowships between participating universities and gas turbine manufacturers. Both are managed by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL). NETL is researching advanced turbine technology with the goal of producing reliable, affordable, and environmentally friendly electric power in response to the nation's increasing energy challenges. With the Hydrogen Turbine Program, NETL is leading the research, development, and demonstration of these technologies to achieve power production from HHC fuels derived from coal that is clean, efficient, and cost-effective; minimizes CO_2 emissions; and will help maintain the nation's leadership in the export of gas turbine equipment.

Project Description

This project will result in a detailed database of flame speed and kinetic information and demonstrate the validity of a comprehensive kinetics model that can predict NO_x formation, flame speed, and ignition behavior in the presence of high levels of dilution and minor levels of likely contaminants. This will lead to a deeper understanding of the turbulent flame speed behavior and NO_x-formation kinetics of HHC fuels for integrated gasification combined cycle (IGCC) power plant applications. The technical approach for achieving this involves coordination with industry representatives in conjunction with a careful series of experiments using flame speed and shock-tube research facilities. The flame speed data will be obtained using two constant-volume vessels. Turbulent-burning velocities at elevated pressure will be obtained in a facility that will be modified to provide a controllable and repeatable level of turbulence. The laminar-burning velocities of mixtures with high levels of water and other diluents will be obtained with

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PARTNERS

None

PROJECT DURATION

Start Date	End Date
10/01/2010	09/30/2013

COST

Total Project Value
$627,212

DOE/Non-DOE Share
$501,712/$125,500

AWARD NUMBER

FE0004679

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a heated flame speed vessel. All experiments will be compared to a comprehensive kinetics model based on prior work of the principal investigator and collaborators. This mechanism will be extended to include a NO_x model taken originally from the literature and improved in several ways, including careful examination of five distinct mechanistic pathways for NO_x formation involving various reactive intermediates, including the NNH mechanism where the planned research will measure rate coefficients that have not been previously reported in the literature. The overall validation and improvement of the comprehensive NO_x mechanism will come from shock-tube ignition tests with advanced diagnostics for recording species-time histories of reactive intermediates, and unique experiments where syngas/HHC fuels are doped with additional species to more rigorously test global mechanisms over a wide range of conditions.

Goals and Objectives

There are two primary goals for this project: to (1) produce a database of flame-speed and kinetic information, and (2) demonstrate the validity of a comprehensive kinetics model that can predict NO_x formation, flame-speed, and ignition behavior in the presence of high levels of dilution and minor levels of likely contaminants. While laminar flame speeds provide valuable data for the validation of the chemical kinetics and provide some insight into the combustion behavior of real systems, it is the turbulent flame speed that is of practical importance to the design of burners. However, less turbulent flame speed data exist for HHC fuels at gas turbine pressures. In addition, the physics of the relationship between turbulent flame speed and parameters such as turbulence intensity, stretch, and laminar flame speed are complex and not necessarily well understood. Reliable turbulent flame speed data for HHC fuels are therefore needed at practical conditions and this project seeks to carry out a methodical and unique array of experiments and analyses that will lead to a deeper and much-needed understanding of the turbulent flame speed behavior and NO_x-formation kinetics of HHC fuels for IGCC applications. In addition to a comprehensive database and improved understanding of the basic physics and chemistry of syngas in the presence of impurities and high levels of diluents, this project will provide a validated chemical kinetics model that can be utilized for the design of new systems and the improvement of existing ones.

Accomplishments

- Assembled a comprehensive chemical kinetics mechanism containing H_2, CO, hydrocarbon, and NO_x chemistry using mechanisms from the literature that were validated at elevated pressures.

- Performed laminar flame-speed measurements of H_2-O_2 mixtures at 1 atmosphere (atm) using the new high-speed camera purchased under this project; these hydrogen measurements will be used as a baseline for comparing mixtures containing CO, diluents, and contaminants.

- Performed ignition delay time measurements of a baseline series of H_2-O_2-argon experiments over a range of pressures from 1 to 30 atm, as well as baseline series of H_2-CO-O_2-argon experiments that are needed for subsequent evaluation of diluents and trace species.

- Determined the effect of nitrogen dioxide (NO_2) and nitrous oxide (N_2O) addition on the ignition of H_2 mixtures using shock-tube ignition experiments. The results were compared to the kinetics mechanism with good results. The NO_x compounds accelerated the ignition process in some cases, but in other cases, particularly at pressures near 1 atm, the NO_x had no effect on ignition delay time.

- Constructed a mock-up rig using Plexiglas® to optimize the turbulence generation system, so the best configuration can be ascertained prior to modifying the existing high-pressure flame speed vessel for the turbulent flame speed measurements.

- Completed a design-of-experiments matrix of laminar flame speeds over a range of H_2-CO mixtures with high levels of water dilution (up to 15% by volume); pressure ranged from 1 to 10 atm, with initial temperatures of 323 or 423 Kelvin (K). Comparison with the chemical kinetics model shows good agreement between data and model.

- Designed and fabricated the turbulent flame speed vessel. This new design used an existing vessel originally designed for laminar flame speeds and added a motorized fan system using the data from the mock-up rig as a guide.

- Obtained turbulent flame speed data for pure H_2 and 50/50 CO/H_2 fuels at 1 atm at a fixed value for velocity fluctuation and turbulence length scale. Correlations of the turbulent flame speed were constructed.

- Performed shock-tube measurements of ammonia-oxygen mixtures in argon over a range of pressures and temperatures and assembled a chemical kinetics model for NH_3 oxidation.

- Measured ignition delay times of hydrogen-oxygen mixtures tainted with various levels of hydrogen sulfide (H_2S) and assembled a chemical kinetics mechanism for H_2S.

- Developed and demonstrated an optical diagnostic for measuring OH concentrations in a shock tube using light absorption near 310 nm. The system using a uv lamp as the light source and a monochromator for spectral selectivity. OH time histories were obtained at 2 and 13 atm in H_2-O_2 mixtures highly diluted in argon.

Benefits

This UTSR project supports DOE's Hydrogen Turbine Program that is striving to show that gas turbines can operate on coal-based hydrogen fuels, increase combined cycle efficiency by three to five percentage points over baseline, and reduce emissions. This project aids in the understanding of turbulent flame speed behavior and NO_X-formation kinetics of HHC fuels for IGCC applications and will support turbine design in power systems utilizing HHC syngas fuel.

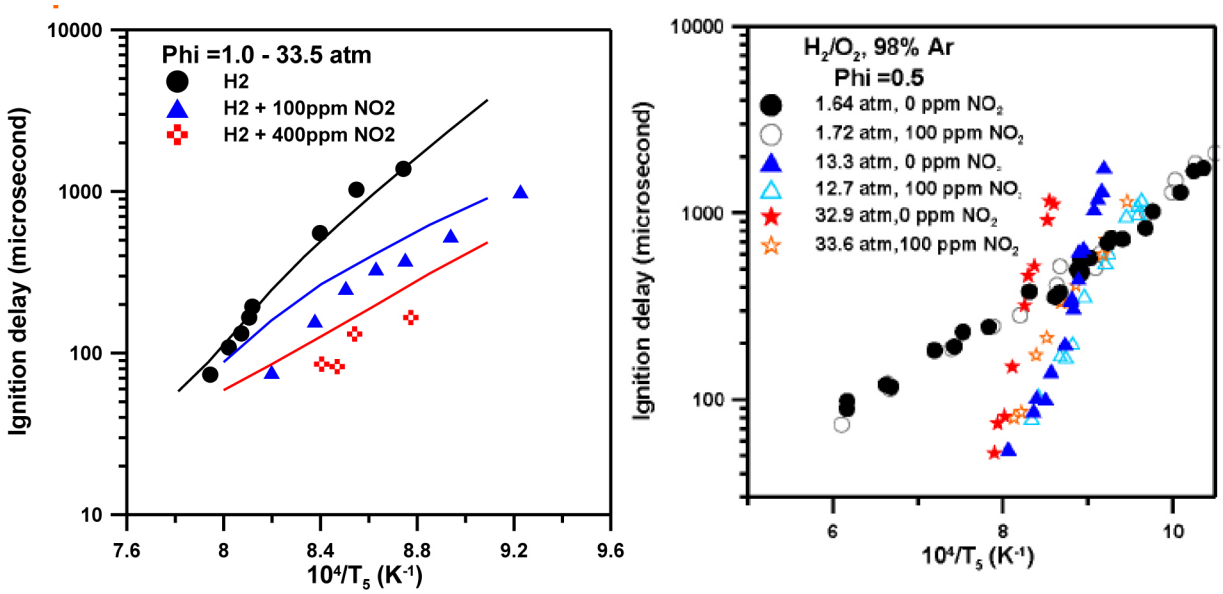

Figure 1a

Figure 1b

Figure 1. Measured ignition delay times of a hydrogen-oxygen mixture with 98 percent argon, with and without NO_2 addition, compared to kinetics model (lines). Figure 1a shows results at a constant 33.5 atm. pressure and 1.0 equivalence ratio (phi), while Figure 1b shows ignition delay results as a function of pressure (from 1.6–33.6 atm.) and constant 0.5 equivalence ratio.

Figure 2. Texas A&M shock-tube test facility being used to elucidate detailed NO_X mechanism chemistry.

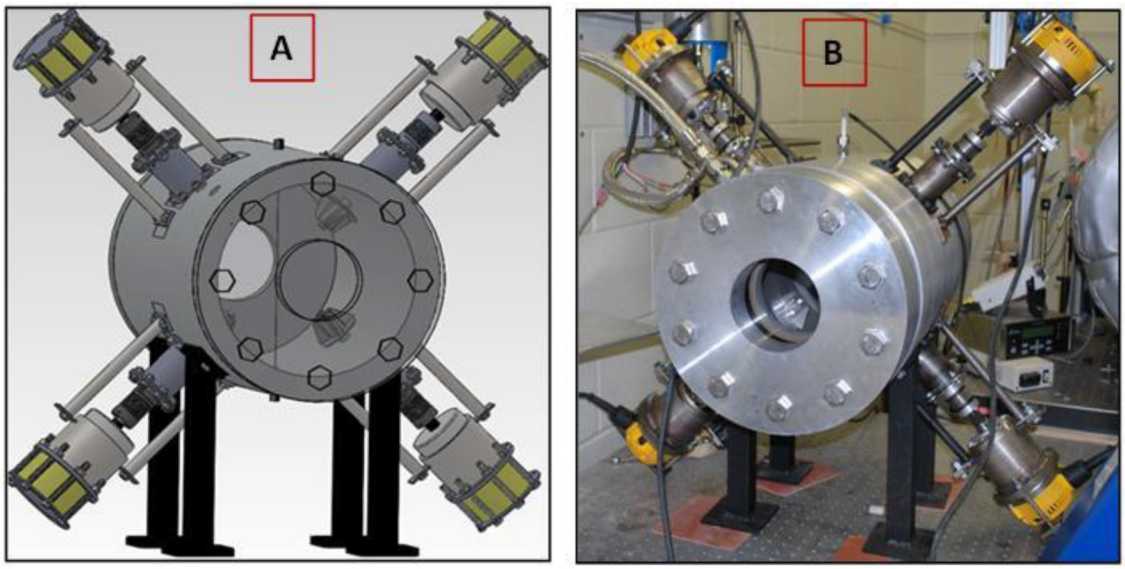

Figure 3. Fan-stirred flame speed vessel. (a) 3D solid works model (b) photograph of the facility. The four fans at the central circumference generate homogeneous and isotropic turbulence at the vessel center.

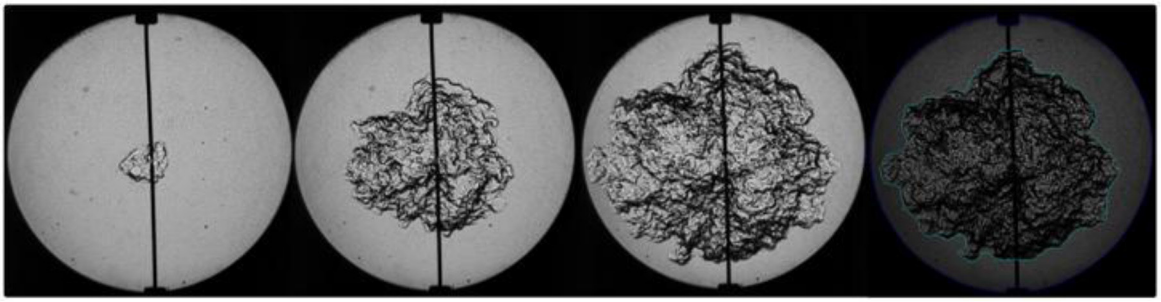

Figure 4. (a-c) Sample images from a typical turbulent flame speed experiment for a 50/50 H_2/CO mixture in air at 1 atm pressure. (d) Image processing technique used to estimate the flame radius by computing the enclosed area within the kernel boundary.

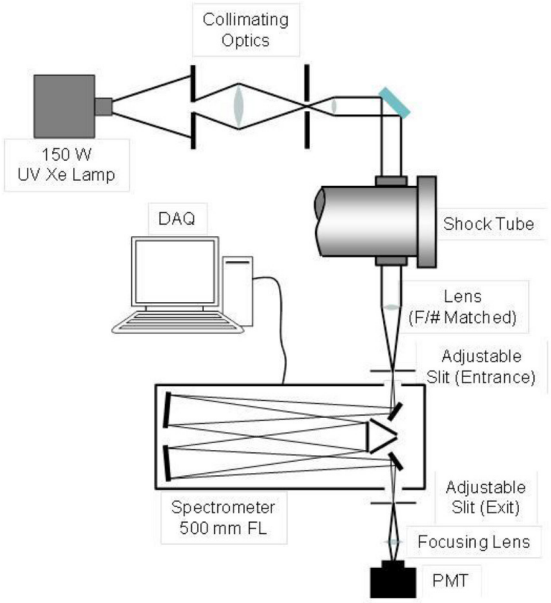

Figure 5. General schematic of OH measurement diagnostic utilizing a 0.5 m focal length spectrometer configured as a monochromator.

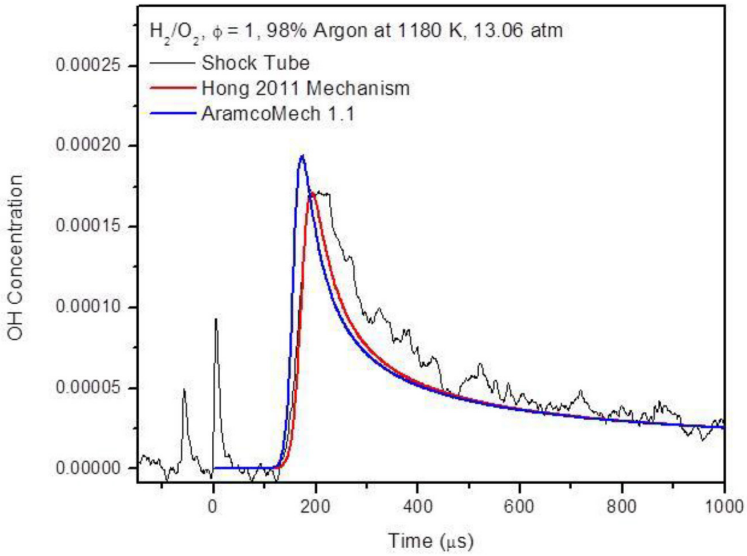

Figure 6. Shock-tube data comparison for OH with two mechanisms for a high pressure H_2/O_2 mixture diluted in argon. Measurement was taken in a shock tube using the new absorption setup (Fig. 5) at TAMU. Conditions correspond to reflected-shock temperature (1180 K) and pressure (13.06 atm) for a stoichiometric H_2-O_2 mixture in argon. Comparison with chemical kinetics mechanisms is good.