DOE FACT SHEETS
FOR
UTSR PROJECTS

Autoignition Studies of Syngas and Hydrogen (SGH) Fuels

FACT SHEET

I. PROJECT PARTICIPANTS

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II. PROJECT DESCRIPTION

A. Objectives

The objective of this project is to parametrically determine the autoignition delay time for CO/H_2 mixtures as function of CO concentration, equivalence ratio, pressure and temperature. The effect of water concentration on autoignition will be determined using mixtures of $CO/H_2/H_2O$. Measurements will be made for operating pressures up to 3.0 MPa and 950 K and typical air mass flow rates of 0.5 kg/s. Since syngas and SGH fuels have varying concentrations of CO, H_2, H_2O, CO_2 and other gases depending on the specific conditions used in producing these fuels, this study has as its objective to provide a fundamental set of data on autoignition under well characterized concentration conditions that represent rapidly mixed conditions. Actual gas turbine engines will be characterized by less well controlled mixing processes and will have fuel/air equivalence (mixture fraction) variations. Thus, the present study aims to provide a basis set of autoignition times that can be universally applied to a broad range of injectors and premixing approaches in which operating conditions vary over the range of conditions measured in this study.

B. Background/Relevancy

Background. The renewed interest in coal-based integrated gasification combined cycle (IGCC) plants is due to the desire for greater fuel supply flexibility and the large known resources of coal in the United States. Current Department of Energy plans strive for efficient, environmentally clean IGCC technologies that can provide both electrical generation and hydrogen production capabilities. Combustion of syngas produced from the coal gasification process, as well as a broader range of syngas and hydrogen (SGH) fuels, has been identified as a key technology area.

Autoignition is a process, not a property of a combustible mixture and, thus, involves a number of variables and parameters that are specific to the mixture, its thermodynamic state and the measurement environment. A succinct definition of autoignition can be stated as "Autoignition is a spontaneous process where by a combustible mixture undergoes chemical reaction leading to the rapid liberation of energy at a rate sufficient to sustain combustion in the absence of an external energy source such as a flame or spark". For a gaseous system, one can view the autoignition process to be a reactants mixing process with a concurrently occurring chemical kinetic reaction process that leads to a rapid release of energy. The characteristic times for the mixing and chemical reaction processes can vary widely for different combustion devices because of different initial conditions in terms of equivalence ratio, pressure, temperature and initial flow velocity. Thus, one must be careful in utilizing autoignition data obtained under different experimental conditions to be sure that the dynamic relation between mixing and chemistry is appropriately captured in the measurement technique.

For the present study, the objective is aimed at characterizing conditions that are typical of lean premixed gas turbine engines as employed currently in electrical power generation. The temperature and pressure conditions relevant to such studies lend themselves to flow reactor studies (see Fig. 1). The reason for this statement lies in the temperature and pressure regime of interest, which usually extends to high pressures, 3 MPa, and temperatures not in excess of 1000 K. A key aspect of the problem is to provide rapid mixing that is well characterized directly downstream of the fuel and air injectors. Furthermore, the flow conditions along the reactor must also be well known in terms of velocity, residence time and temperature.

Relevancy: From an operations standpoint under IGCC conditions to meet gas turbine fuel demand requirements, the fuel composition will vary as a function of the gasifier operating levels. Clearly, this introduces new challenges to gas turbine technology since fundamental characteristics of SGH fuels related to autoignition, flashback and blowout are presently not available. This three year program is geared towards systematically examining autoignition phenomena related to SGH fuels at the high pressure, temperature and flow velocity conditions representative of actual gas turbine operating conditions and determine the autoignition time as a function of composition, pressure and temperature. This information will provide a fundamental basis from which design gas turbines that can handle fuel composition variations over a wide range of conditions.

C. Period of Performance. 8/01/2005to 7/31/2008

D. Project Summary

Under the University Turbine Research (UTSR) program, *The Pennsylvania State University* is undertaking a three year program to measure the autoignition temperature of $CO/H_2/H_2O$ as a simulant for syngas. In the first two years, autoignition delay times will be determined over a range of conditions for CO/H_2 fuel mixtures ranging from pure syngas [$CO+3H_2$] to pure hydrogen [H_2]. Autoignition characteristics of $CO/H_2/H_2O$ fuels also will be investigated. For the autoignition studies involving CO/H_2 fuel mixtures, CO concentration in fuel will be varied between 0 (pure H_2) and 25% (pure syngas), the equivalence ratio will be varied from 0.3 up to 1.0, pressure and temperatures will range up to 3.0 MPa and 950 K, respectively, and mean flow reactor velocities are expected to be between 10 and 40 m/s. Experimental conditions for the effort involving $CO/H_2/H_2O$ fuels will be determined based on the results obtained in the first two years of the effort.

III. PROJECT COSTS

$419,036

IV. MAJOR ACCOMPLISHMENTS SINCE BEGINNING OF PROJECT

- Define experiments in terms of hardware geometry and flow conditions for first set of autoignition characterization experiments involving pure syngas and pure hydrogen fuels.
- Completed initial comparison for current chemical kinetic models to predict autoignition and compared to available date (see Fig. 2).
- Final hardware design complete July 2006.

V. MAJOR ACTIVITIES PLANNED DURING THE NEXT 6 MONTHS

- Initiate autoignition experiments for pure syngas fuel as a function of pressure (1.0-3.0 MPa) and temperature (up to 800 K) for multiple velocity conditions (10-40 m/s).

VI. MAJOR ACCOMPLISHMENTS PLANNED IN OUTYEARS (6-18 MONTHS)

- Conduct autoignition experiments for pure hydrogen fuel as a function of pressure (1.0-3.0 MPa) and temperature (up to 950 K) for multiple velocity conditions (10-40 m/s).
- Develop global reaction rate formulation for CO/H_2 fuels. Initiate chemical kinetics modeling using plug flow reactor and CHEMKIN^{TM} program.
- Analyze and document first set of autoignition results for pure syngas and pure hydrogen fuels. Post results on website.
- Based on the results obtained in Year 2, define experiments in terms of hardware geometry and flow conditions for second set of autoignition characterization experiments involving three or four CO/H_2 fuel mixtures between pure syngas and pure hydrogen fuels.

VII. ISSUES

None

VIII ATTACHMENTS

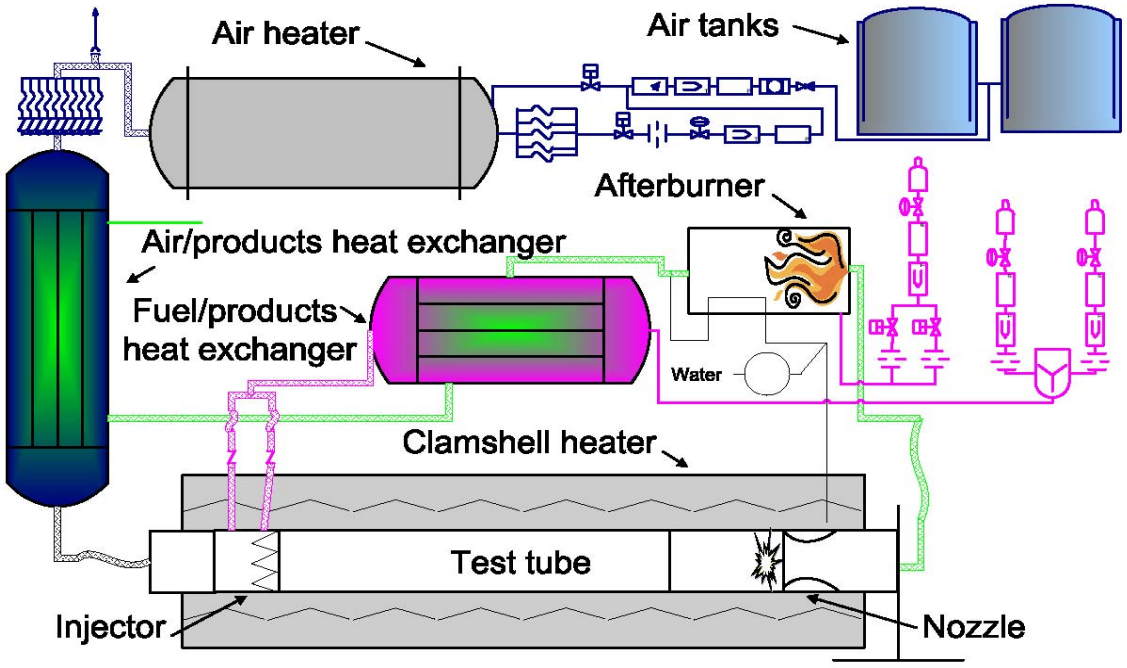

Fig. 1. Schematic of high-pressure autoignition test rig.

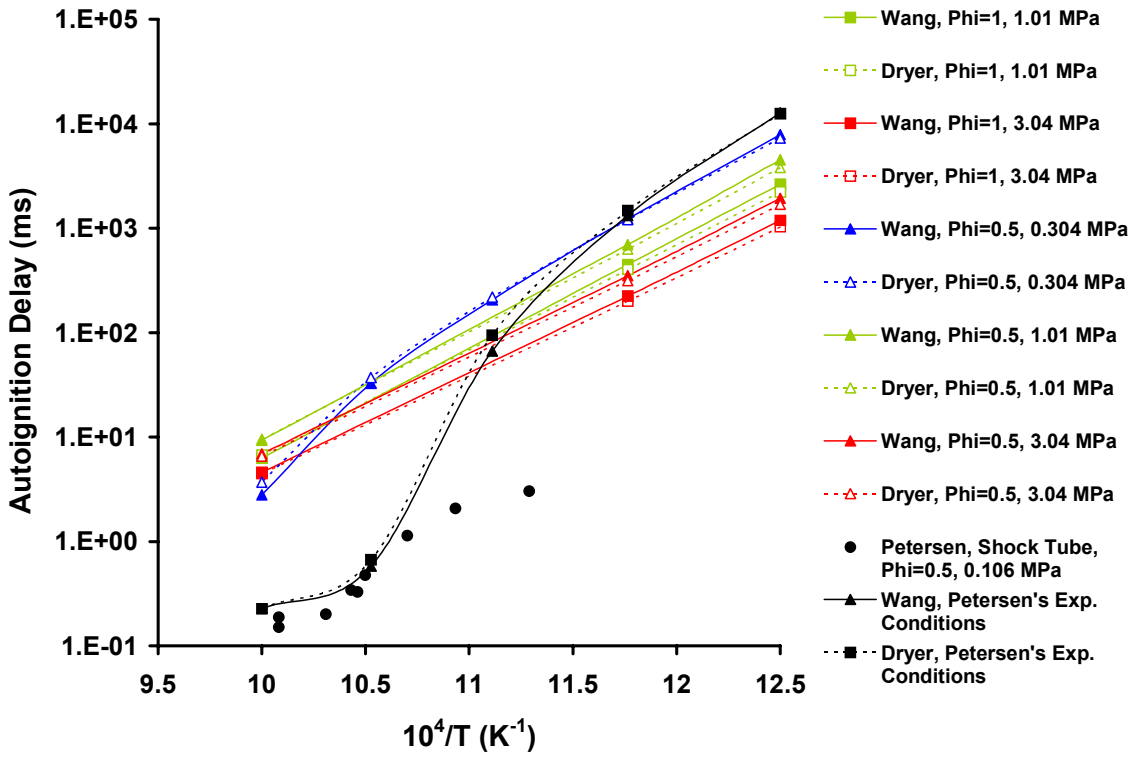

Fig. 2. Autoignition delay for a H_2/CO/Air mixture (fuel is $[CO + 3H_2]$). $\phi = 1$ and 0.5; P = 0.106, 0.304, 1.01 and 3.04 MPa (15.4, 44.1, 147 and 441 psia); Wang and Dryer mechanisms.