COMPUTATIONAL AND EXPERIMENTAL STUDY OF JET FUEL COMBUSTION

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SUMMARY/OVERVIEW

A coordinated experimental and computational program is needed to develop chemical models of jet fuel that can be used within a larger research and development program. In this proposal we will initiate a joint experimental and computational program designed to test the feasibility of surrogate formulations of JP-8 capable of matching overall properties of the complex fuel and more detailed aspects of its combustion, such as flame structures. The work proposed herein will be leveraged on complementary research at the University of Utah and the University of Milan (Italy). The work will help establish a research infrastructure to provide a better understanding of the combustion of jet fuel, to the benefit of both commercial and military users.

TECHNICAL DISCUSSION

With a starting date of 2/15/06, we initiated a joint experimental and computational program designed to test the feasibility of surrogate formulations of JP-8 capable of matching overall properties of the complex fuel and more detailed aspects of its combustion, such as flame structures. Once the surrogate is identified, its kinetic behavior will be modeled and, after additional validation, the model will be reduced to a sufficiently small subset of critical kinetic reactions to be incorporated in realistic computational codes. Specifically, a comprehensive campaign of measurements and computations in prototypical flame environments, such as premixed flames and diffusion flames will be undertaken which will include measuring and computing global properties such as laminar flame speeds, S_L, extinction strain rates, a_{ext}, and ignition strain rates, a_{ign}. We will also compare flame structure including the temperature and gaseous hydrocarbons up to C_{12}. All of the above would be studied as critical variables, such as inlet temperature, composition, overall mixture equivalence ratio, vitiation equivalence ratio and pressure are varied.

Experimental Approach

A counterflow burner will be the workhorse of the experimental activity. A schematic of the counterflow experimental setup is shown in Figure 1. It uses a carefully contoured geometry to ensure flow uniformity at the burner mouths. Experiments can be

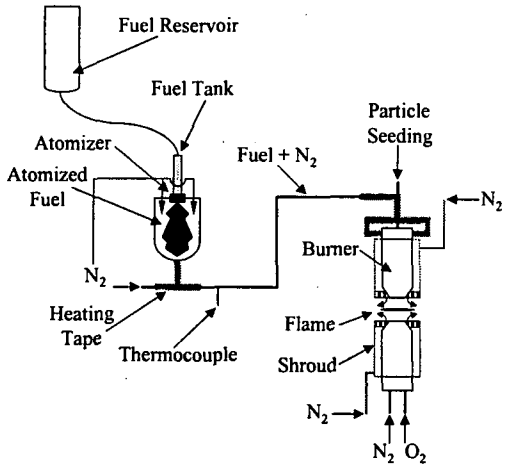

Figure 1. Schematic of the nonpremixed counterflow JP-8 configuration.

conducted with a fuel mixture introduced from the upper burner, in order to benefit from the heating of the exhaust gas and reduce the risk of condensation, and an oxidizer mixture introduced from the lower burner. The fuel and oxidizer inlet concentrations can be chosen to inhibit the formation of soot, a particularly significant advantage of this configuration when using fuels prone to soot such as those under consideration. Typically, overall fuel-lean flames will be examined. Furthermore, to enhance the flame stability and prevent soot formation at the interface of the flame with the room air, a shroud flow of N_2 is provided. The fuel side is maintained at a temperature above the dew point of the nitrogen-diluted fuel mixture admitted into the burner. The flow rates of the reactant streams are measured using mass flow controllers.

The vaporization of the liquid fuel is a critical issue. For the multicomponent mixture, to avoid fractional distillation, an ultrasonic nebulizer, capable of generating rapidly vaporizing droplets a few microns in diameter, is used to introduce liquid fuel droplets into a heated nitrogen stream, yielding complete vaporization. This vaporized fuel/inert mixture is then conveyed to the burner through a heated tube maintained at elevated temperature and monitored via thermocouples. Temperature measurements are obtained using coated Pt/10%Pt-Rh thermocouples. The measurements will be corrected for radiative losses using both spherical and cylindrical geometries. The thermocouple probe is custom-designed to minimize perturbations on the low strain velocity field.

Premixed flame studies will be conducted in a modification of the counterflow configuration. In principle, premixing the feed streams and splitting them between the two burners with valves on each line to match pressure drops, would make the experimental system suitable for the "twin flame" approach to the measurement of flame speeds [2] and flammability limits. This approach is very appealing because of its inherent adiabaticity, but is potentially affected by uncertainties in the extrapolation of the measured flame speeds to zero strain, although with large nozzle separations these uncertainties are perhaps acceptable. A more recent technique that can be easily implemented in our set-up relies upon using the transition from planar to conical Bunsen flames in a jet/wall configuration [3]. Detailed work from the same group has shown that at low strain rates the flame is affected minimally by the wall [4]. We have recently begun experimenting with the set-up in Figure 2 and it appears to work well except under very lean conditions. As a result, we will apply both approaches, each with its own advantages, both being aerodynamically "clean."

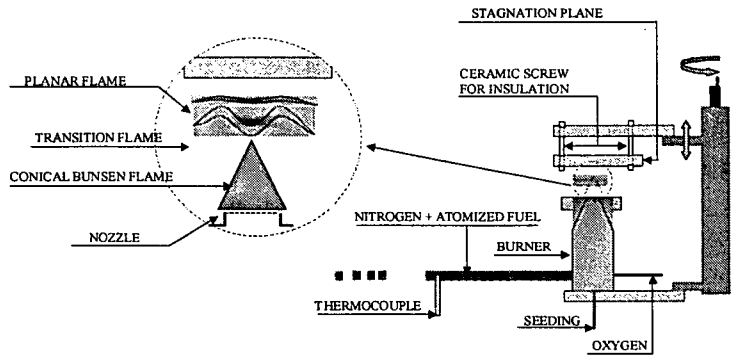

Figure 2. Schematic of the premixed counterflow JP-8 configuration.

Computational Methodology

The form of the governing equations for both the freely propagating and counterflow flame models are well documented. In the freely propagating case, conservation equations for the species and energy are solved together with an equation for the mass flow that is formulated in terms of an eigenvalue problem for the adiabatic flame speed. The counterflow problem is modeled by considering a similarity solution of the two-dimensional conservation equations of mass, momentum, species and energy, valid along the stagnation point streamline. In both problems, the resulting set of equations can be written in terms of a nonlinear boundary value problem on a fixed spatial domain.

Of inherent importance to both the premixed and nonpremixed studies will be the ability to vary one or more quantities as the remaining system parameters are held fixed. For example, in the premixed problems we are interested in allowing the equivalence ratio to change as the pressure and inlet temperature are held fixed or we may want to vary the inlet temperature as the pressure and equivalence ratio are fixed. For the diffusion flames, the strain rate, inlet mass flow rates and temperatures are parameters of interest. While we could compute a single flame with specified values of these parameters and then use this computed solution as a starting estimate for a new problem with different parameter values, this is extremely inefficient. Instead, we will apply a continuation method such that the grid and the solution smoothly change as the parameter is varied.

Once a solution to the flame equations has been obtained, it is often useful to investigate those parameters to which the solution is most "sensitive" (see, e.g., [5]). In the past, however, the major obstacle in obtaining sensitivity information systematically was the additional amount of computation required for solving the sensitivity equations. An advantage of solving the premixed and counterflow flames by a Newton based method is that first-order sensitivity information can be obtained at a fraction of the cost of the total calculation [6]. Critical parameters to be investigated include reaction rate and transport coefficients as it is important to understand whether the agreement, or lack thereof, of global properties and flame structure is originating from the kinetics of the surrogate or the transport properties employed.

In parallel with the proposed experimental program, we will initiate a process to reduce the surrogate mechanism. We envision the procedure occurring in several stages due, in part, to the large number of chemical species (> 220) and the large number of elementary chemical steps (> 5000) in the surrogate formulation. The first stage of the reduction process would generate a "skeletal" mechanism—one which is significantly reduced in the number of chemical species and reactions from the parent mechanism but one that is still untenable for use in a turbulent reacting flow model. The mechanism can be reduced further by employing a steady-state analysis ultimately leading to a system so that partial equilibrium and truncated steady-state approximations can be used to produce a mechanism that we envision will be small enough to be computationally effective in turbulent reacting flow models. An alternative approach includes the intrinsic low dimensional manifold method (ILDM) [7]. No reduction process involving flames has been attempted on a mechanism as large as the one proposed herein and, hence, the tradeoffs between the two reduction methodologies need to be assessed in practical computations before one method is recommended over the other. We point out that the specific level of the reduction process will depend upon what parameters the reduced mechanism will be required to reproduce. For example, if one wants to match soot volume fractions and radiation levels, significant species reduction may not be as viable compared to matching peak temperatures and flame speeds.

We will discuss results obtained in the counterflow diffusion flame briefly [8] and system modifications since the grant's inception

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