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Computational and experimental study of JP-8, a surrogate, and its components in counterflow diffusion flames

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Abstract

Non-sooting counterflow diffusion flames have been studied both computationally and experimentally, using either JP-8, or a six-component JP-8 surrogate mixture, or its individual components. The computational study employs a counterflow diffusion flame model, the solution of which is coupled with arc length continuation to examine a wide variety of inlet conditions and to calculate extinction limits. The surrogate model includes a semi-detailed kinetic mechanism composed of 221 gaseous species participating in 5032 reactions. Experimentally, counterflow diffusion flames are established, in which multicomponent fuel vaporization is achieved through the use of an ultrasonic nebulizer that introduces small fuel droplets into a heated nitrogen stream, fostering complete vaporization without fractional distillation. Temperature profiles and extinction limits are measured in all flames and compared with predictions using the semi-detailed mechanism. These measurements show good agreement with predictions in single-component *n*-dodecane, methylcyclohexane, and iso-octane flames. Good agreement also exists between predicted and measured variables in flames of the surrogate, and the agreement is even better between the experimental JP-8 flames and the surrogate predictions.

Keywords: Surrogate; JP-8; Simulation; Counterflow diffusion flames

1. Introduction

The study of the combustion processes in practical aero-combustors is an essential tool to characterize and improve combustor efficiency and to identify and eliminate those mechanisms leading to pollutant formation. However, the numerical and experimental study of these processes in practical situations is daunting from two perspectives. The first challenge stems from the fact that aviation fuels, such as JP-8 and kerosene, are mixtures of a large number of hydrocarbons that together must meet standardized specifications. Due to the variability of composition, kinetic studies of such fuels can only be based on a "surrogate" mixture of well-known hydrocarbons that

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possesses thermochemical properties similar to those of the fuel under study. The kinetic mechanisms that describe such surrogate mixtures often consist of hundreds of gaseous species participating in thousands of reactions. From a computational perspective, these large mechanisms increase both the size and complexity of an already stiff set of strongly coupled, highly non-linear partial differential equations. A second challenge arises from the fact that combustion in practical aero-combustors, whether non-premixed or partially premixed, is certainly turbulent and inherently multidimensional. By some estimates, the direct numerical simulation (DNS) of turbulent combustion will exceed computational capabilities for at least 20 years [1]. However, there are computationally feasible alternatives that give substantial insight into the chemical and physical processes in turbulent flames while also allowing for the examination of complex chemistry and detailed transport in numerically and experimentally tractable configurations. One such configuration is the counterflow diffusion flame, an established tool with which to examine the interactions between detailed transport and complex chemistry, and one that affords good opportunities for comparison between computation and experiment.

A number of investigations have addressed the challenge of formulating surrogate blends for aviation fuels and developing the necessary kinetic mechanisms for these blends. The oxidation of these multicomponent mixtures has been studied computationally and experimentally in jet-stirred reactors for both two-component [2,3] and three-component surrogate mixtures [4] and in rich, premixed flames for a two-component surrogate mixture [3,5,6]. In contrast, there exist relatively few computational or experimental studies of the combustion of aviation fuels under non-premixed conditions. One recent example examines a counterflow kerosene diffusion flame computationally using a detailed kinetic mechanism for a two-component surrogate mixture [3].

As part of a broader effort to validate chemical kinetic models of multicomponent surrogates in a variety of combustion environments, we examine counterflow diffusion flames computationally and experimentally using both a six-component JP-8 surrogate blend and individual surrogate components as fuels. Experimentally, a non-sooting diffusion flame is stabilized between counterflowing, nitrogen-diluted streams of fuel and oxygen. Temperature profiles and extinction limits are measured for each flame and are compared against predicted values obtained using a two-point boundary value solver and a semi-detailed kinetic model developed for the six-component surrogate. Preliminary results were presented in [7].

2. The surrogate

The present study models JP-8 as a six-component blend of well-known hydrocarbons with the following molar composition: 10% iso-octane (C_8H_{18}), 20% methylcyclohexane (C_7H_{14}), 15% *m*-xylene (C_8H_{10}), 30% *n*-dodecane ($C_{12}H_{26}$), 5% tetralin ($C_{10}H_{12}$), and 20% tetradecane ($C_{14}H_{30}$). This surrogate blend accurately simulates the volatility and smoke point of a practical JP-8 fuel [8]. The semi-detailed kinetic mechanism for this surrogate blend is based on an existing hierarchically constructed kinetic model for alkanes and simple aromatics extended to account for the presence of tetralin and methylcyclohexane as reference fuels [8,9]. This mechanism has been previously validated by comparing numerical simulations with experimental results for individual surrogate components in plug flow reactors and rich premixed flames as well as with experimental data for rich, premixed kerosene flames [8].

3. Numerical methods

We use the elliptic form of the two-dimensional conservation equations to model the gas-phase counterflow diffusion flame, shown schematically in the inset of Fig. 1. The result is a strongly coupled, highly non-linear set of $K + 4$ partial differential equations in cylindrical coordinates, where K is the number of gas-phase species. A similarity solution valid along the stagnation streamline reduces the complexity of the problem [10]. This assumption reduces the set of non-linear partial differential equations in two dimensions to a set of non-linear ordinary differential equations valid along the stagnation streamline. The problem is then closed with the ideal gas law and the application of appropriate boundary conditions, including a plug flow velocity boundary condition at both inlets. Local properties are evaluated using vectorized and highly optimized transport and chemistry libraries [11].

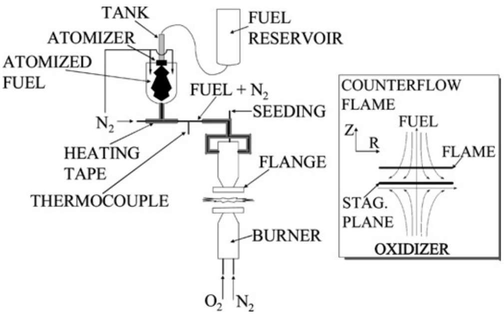

Fig. 1. A schematic diagram of the experimental setup, with an inset diagram of the counterflow diffusion flame.