Final Report
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Partially-Premixed Flames in Internal Combustion Engines
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Program scope

The purposes of this joint university-industry research program are: 1) to use advanced laser diagnostics and detailed chemistry models to understand partially-premixed flames in unique laboratory burners, 2) to use advanced laser diagnostics to observe and characterize partially-premixed combustion in optically-accessible direct injection gasoline engines, and 3) to more fully develop laser diagnostic techniques for temperature and flame front imaging in partially-premixed flames and IC engines. The work is being done primarily at Vanderbilt University, General Motors Research and Development Center, and the University of Michigan.

The goals of this research are 1) a better understanding of the effects of strain and curvature on partially-premixed flame structure, 2) better conceptual models of partially-premixed combustion in highly stratified direct injection engines for automotive applications, and 3) improved and more robust laser diagnostic methods for use in university and industrial environments.

Vanderbilt University

At Vanderbilt, planar and curved stretched flames were measured and computed to understand the effect of stretch and curvature on the chemistry of partially premixed flames. Measurements of species concentrations and temperature were made with visible Raman scattering and compared to complex chemistry, detailed transport calculations of the same flames. A visible laser-based Raman system was developed to obtain relatively-interference-free Raman signals in hydrocarbon and hydrogen flames (Osborne et al. 2000). Figure 1 shows a schematic of this system, which uses a frequency-doubled, Q-switched Nd-YAG laser as the Raman excitation source and a cryogenically-cooled CCD as the detector. The system was first applied to measure planar flames of hot products vs. lean propane/air reactants (Cheng et al. 2002a; Wehrmeyer et al. 2001, 2002) and methane air/reactants (Cheng et al. 2002b, 2003; Wehrmeyer et al. 2003) as sketched in Fig. 2.

Fig. 1: Schematic of visible Raman system using cryogenically-cooled CCD camera.

Fig. 2. Opposed jet flames of lean methane-air mixtures vs. hot products from a H₂-air flame. a) “Positive flame speed” flame. b) “Negative flame speed” flame.

These opposed jet flames were chosen to simulate what is expected to occur in a stratified-charge direct injection spark ignition (DISI) engine, where hot products impinge upon a zone of either lean or rich reactants. For lean hydrocarbon mixtures, either a “positive flame speed” (Fig. 2a) or a “negative flame speed” flame (Fig. 2b) may form.

Fig. 3. Experimentally-measured and numerically-predicted structure of planar flame produced by $\phi = 0.68$ methane air jet impinging on $\phi = 0.28$ hydrogen-air jet. $\tau = 140 \text{ sec}^{-1}$. Numerical simulations shown for four different reaction mechanisms.

Fig. 4. Experimentally-measured and numerically-predicted structure of planar flame produced by $\phi = 0.54$ methane-air jet impinging on $\phi = 0.28$ hydrogen-air jet. $\tau = 140 \text{ sec}^{-1}$. Numerical predictions obtained using GRI-Mech 3.0.

The low strain-rate, positive-flame speed flame sketched in Fig. 2a was measured and calculated as shown in Fig. 3 (Wehrmeyer et al. 2003). Here the lean methane-air flame forms on the methane-air side of the stagnation plane and propagates against the methane-air jet. The

measurements of flame temperature and concentrations are compared to four different chemical mechanisms: the C1 and C2 mechanisms (Peters 1993), Williams mechanism (Williams 2003) and GRI Mech 3.0 (Smith et al. 1999). All the mechanisms compare fairly well although the C1 mechanism under-predicts the flame speed of the lean methane-air flame.

The “negative flame speed” flame sketched in Fig. 2b is measured and the results are shown in Fig. 4. Here the lean methane-air flame is so weak that the reaction is now occurring on the H_2 -air side of the stagnation plane. The methane fuel diffuses across the stagnation plane and burns in the hot products from the H_2 -air flame. This is a so-called “negative flame speed” flame. Only the GRI Mech 3.0 simulation results are shown as the numerically predicted results are essentially the same for all four reaction mechanisms.

Curved, premixed H_2 -air “tubular” flames have been examined to determine the effect of curvature and stretch on premixed flames. A unique tubular burner was developed at Vanderbilt (Mosbacher et al. 2001, 2002a, 2002b; Wehrmeyer et al. 2001, 2003) that allowed for optical access. Previous tubular burners had very limited optical access. Figure 5 shows schematics of the Vanderbilt tubular burner. A premixed combustible mixture is introduced to the outer circular chamber via a plenum with 16 circumferentially spaced inlet ports. The reactant mixture diffuses through fine gauge stainless steel wool (used to provide a uniform radial pressure drop in the flow chamber) and exits through a converging cylindrical nozzle of 1.5 cm radius and 2 cm height. A premixed tubular flame, with products exiting radially inward from the flame and the reactants flowing radially inward toward the flame, is formed around the cylindrical axis of the burner. The flame location is the radial position where the burning velocity balances with the upstream radial velocity of the unburned mixture. In this manner, premixed tubular flames of

Fig. 5. Schematics of the tubular burner.

various radii can be formed by adjusting the reactant mixture velocity, thus controlling the degree of curvature and aerodynamic straining. A unique feature of the tubular burner is the provision of three optical access ports. Two laser access ports, located at 180° from each other, are 25 mm in diameter. A third 50 mm diameter optical port, located at right angles to the laser ports, is used by the light detection system to collect scattered light.

The axisymmetric flow-field in the tubular burner radially converges and axially diverges. Consequently, the tubular flame is stabilized by a finite rate of stretch. A specific expression for the global stretch rate, $\dot{\gamma}$, in the tubular flame can be derived (Matalon 1983) and is given as,

$$\dot{\gamma} = \frac{2V}{R},$$

where V is the radial inlet velocity, and R is the nozzle radius (1.5 cm).

In order to numerically model premixed tubular flames, the standard Oppdif program (Kee et al. 1999) was modified to account for the radial geometry. Oppdif normally models opposed jet flames of axial symmetry, where the reactants originate along the symmetry axis and exit radially away from the axis. Flame structure is then mapped onto the axial dimension. In a tubular flame, the radial coordinate, instead of the axial coordinate, is used as the spatial dimension through which flame structure is mapped. By transforming the spatial coordinate and seeking a similarity solution of the two-dimensional conservation equations, the tubular flame can be modeled as a two-point boundary value problem. For this current work, the Oppdif program was modified for the tubular flame geometry (Mosbacher et al. 2002b).

Numerical simulations for the experimental premixed H_2 -air tubular flames examined were performed with detailed transport and complex chemistry. Several H_2/O_2 chemical kinetic mechanisms were examined. Gas phase radiation in the optically-thin limit was assumed.

Fig. 6. Comparison of predicted temperature profiles from four reaction mechanisms in a premixed H_2 -air tubular flame ($\dot{\gamma}=0.175$, $\dot{\gamma}=90 \text{ s}^{-1}$).

Figure 6 shows a comparison of Raman temperature measurements with numerical simulations using four different chemical kinetic reaction mechanisms including thermal diffusion effects. Data from both sides of the tubular flame centerline are plotted versus radius to illustrate the axisymmetric structure of the flame. The adiabatic equilibrium flame temperature is also shown by the horizontal line at ~ 875 K to emphasize thermal-diffusion/curvature effects. Figure 6 is for a flame with a stretch rate of 90 s^{-1} and measured temperature of ~ 1295 K, which is ~ 420 K above the adiabatic flame temperature. Comparison of the mechanisms reveals that the kinetics of Mueller et al. 1999 and Yetter et al. 1991 are the strongest, leading to higher flame speeds, larger flame radii, less fuel focusing, and lower flame temperatures. Reaction mechanism trends illustrated in Fig. 6 are representative of all the stretch rates examined. At higher stretch rates significant differences are detected among the experimental and numerical data sets, indicating low temperature H_2/O_2 chemical kinetics models may need improvements.

In Fig. 7, the flame temperatures for planar and tubular premixed H_2 -air flames are compared vs. stretch rate (Wehrmeyer et al. 2003). Thermal-diffusive effects in highly curved (~ 2 mm flame radius) tubular flames significantly influence flame structure: leading to flame temperature increases of ~ 120 K over the planar unstretched flame temperature (~ 1180 K at $\mathcal{K} = 0$, not shown in Fig. 7). The simulations and measurements of tubular flames compare well below $\sim 120 \text{ s}^{-1}$ but above that value there are significant departures. The experimental observations show extinction occurring ($\sim 227 \text{ s}^{-1}$), while numerical simulations over-predict the extinction limit ($\sim 750 \text{ s}^{-1}$).

Fig. 7. Comparison of flame radius and peak flame temperature vs. stretch for H_2 -air tubular flames of $\mathcal{K} = 0.175$. Numerical simulations and experimental data of opposed jet flames under identical conditions are shown for comparison.

General Motors

At GM R&D (with internal GM funding), partially-premixed flame combustion was studied in stratified-charge DISI engines. A single cylinder engine, with an extended piston that has optical access through a quartz piston window, is used to obtain high-speed video camera images of the stratified charge combustion processes. Figure 8 shows a schematic of the “glass-piston” engine, along with a field-of-view image of the cylinder. Using narrow-band spectral filters, and a three-ICCD camera system, images of the OH^* , CH^* , and C_2^* emission are obtained. The images show the growth of both the combustion zones and the sooting zones as functions of crank angle. In addition, GM established a Satellite Research Laboratory at the University of Michigan, which has provided money and equipment to equip an engine test cell with two DISI single-cylinder engines (one all-metal and one with extensive optical access). GM is funding several graduate students at UM as part of the Satellite Laboratory, as well as funding a UM graduate student as a summer intern at GM R&D. Also chemical kinetic mechanisms that were developed at GM were given to Vanderbilt University to be used in the numerical investigation of partially premixed flames.

At General Motors, graduate students from the University of Michigan (B. Stojkovic) and Vanderbilt University (M. Mosbacher) worked with Drs. Drake and Fansler during the Summer of 2001 to examine ultraviolet and visible combustion emission spectra in a DISI engine for different operating conditions. Drawing on the results of this study, experiments to combine spectrally resolved high-speed combustion imaging (Fansler et al. 2003) with simultaneous spark-emission spectroscopy measurements of local fuel-air equivalence ratio were begun. The spark-spectroscopy technique was originally developed at GM in 2000-2001 with Stojkovic's collaboration under GM funding (Fansler et al. 2002b). Extension and systematic application of this combined approach during 2002 was included in Stojkovic's doctoral thesis (see page 13). A recent report of this work is in Fansler et al. (2002a).

Fig. 8. DISI engine with optical access through the piston.

University of Michigan

An optical direct-injected engine was designed and built-up for imaging experiments on mixing and combustion under stratified charge combustion conditions. The design and setup of the single-cylinder optical direct injected gasoline engine was guided and assisted by GM. This way, the engine setup at UM could duplicate the engine conditions at GM to allow the pursued synergy within this project. B. Stojkovic spent substantial amounts of time at the GM R&D center to get additional training on work with optical engines and implementation of optical diagnostics to characterize partially-premixed combustion in engines. As a primary illumination source for imaging experiments a tunable KrF excimer laser was chosen since it allows excitation of several species of interest: fuel tracers, hydroxyl radicals and nitric oxide. Additionally a Raman shifting cell for tuning range extension was set up.

Quantitative measurements of the fuel distribution in dense high-pressure sprays can be obstructed by substantial laser beam and signal attenuation. These processes were characterized experimentally and numerically (Sick and Stojkovic 2001) to allow an improved measurement of the initial phase of the mixture preparation to partially premixed conditions in DISI engines. In addition to the attenuation of the exciting laser beams, measurements under direct-injected conditions can suffer from severe attenuation of the signal light. A method was developed to measure the signal attenuation in two dimensions that perfectly mimics the signal light's spectral composition. Subsequent work was performed on the temporal and spatial history of a spray event to evaluate the penetration, and atomization for engine geometries (Stojkovic and Sick 2001). This work also addressed interference effects on laser-based measurements in direct injected gasoline engines, as they would influence quantitative studies by producing unwanted signal reflections from nearby surfaces.

Fuel/air equivalence ratio measurements based on planar laser-induced fluorescence (PLIF) of toluene that was added to iso-octane fuel were performed. The level of unmixedness could be characterized in detail from the PLIF images. Figure 9 shows single-shot images of the equivalence ratio near the spark plug to illustrate the large fluctuations from cycle to cycle. Calibration of equivalence ratio measurements was performed by several means. The amount of fuel injected is known from the injector characteristics, and the amount of air trapped in the cylinder could be determined via flow rate measurements using critical orifices. This measurement is confirmed via a commercial lambda meter that was used in the engine exhaust.

Fig. 9. Single-shot images of the equivalence ratio near the spark plug at the time of spark.

A KrF excimer laser was used to produce toluene fluorescence. The fluorescence signals from this excitation scheme exhibit a substantial temperature dependence that has to be taken into account for quantitative measurements. However, two-dimensional in-situ temperature measurements in engines are very difficult and need further development. It had been demonstrated by Einecke et al. (2000) that this can be achieved with a two-line excitation approach. For homogenous fuel distributions one can measure the signal strength as a function of crank angle and hence, temperature and pressure variation. The temperature dependence was characterized and used for image correction purposes (Frieden and Sick 2003a, b, Frieden et al. 2002).

Quasi-3D imaging experiments were performed to investigate the complex mixing and combustion patterns in the engine (see Frieden and Sick 2003a for details). This was accomplished by an automated scanning system that adjusted laser sheet and camera positions. An example of this is shown in Figure 10 for the fuel spray during the injection process to illustrate how the 3D structure changes with changes in in-cylinder engine flow.

Through the combination of two fluorescence tracers (toluene and 3-pentanone) a quantitative strategy for imaging of oxygen in engines was developed and applied for the first time (Frieden et al. 2002). This additional information then allows a complete characterization of the gas contents in the cylinder as now information about residual burnt gases can also be derived. Figure 11 illustrates the result of a study where the engine was operated with and without residual gases. The graphs show how sensitively and accurately the imaging technique can determine this effect.

Fig. 11. Two-tracer imaging results for skip-firing and continuous firing of the engine. Exhaust gas measurements confirm the optical measurements for the bulk exhaust gas. Open symbols show results for the skip-fired operation.

Fig. 10. Average fuel spray image for 2000 rpm, 278 BTDC. Elevations (from top) = 1, 4, 8, 12, 16, [mm] etc. Piston location shown in white.

Fig. 12. Turbulent flame structure in a direct injected engine. The image plane is horizontal, 5 mm below the injector.

The penetration of a turbulent flame front into the unburnt fuel/air mixture is shown in Fig. 12, where a single-shot PLIF image of the fuel visualizes the flame location via the disappearing fuel. Quasi-3D images were also obtained for the combustion phase of the engine cycle for different conditions (see Frieden and Sick 2003a for details)

Nitric oxide formation was studied for different combustion conditions in the optical direct injection engine using NO A-X (0,2) excitation near 247.9 nm. An example is shown in Figure 13 where for overall stoichiometric conditions the internal engine flow was modified from high swirl to low swirl conditions. A marked difference in the formation rate and the NO distribution is visible. This difference is in accordance with the change in flame propagation characteristics that was measured earlier.

Fig. 13. Average nitric oxide distribution near the spark plug for different engine operating conditions.

Publications acknowledging DOE support

- Cheng, Z., Wehrmeyer, J. A., and Pitz, R. W. (2002a) "Opposed Jet Flames of Very Lean or Rich Premixed Propane-Air Reactants vs. Hot Products." Paper presented at the Spring Technical Meeting of the Combustion Institute Central States Section, Knoxville, TN, April 8-9.
- Cheng, Z., Wehrmeyer, J. A., and Pitz, R. W. (2002b) "Opposed Jet Flames of Lean Premixed Methane-Air Reactants versus Hot Products," 38th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Indianapolis, Indiana, Paper No. AIAA-2002-4021, July 7-10.
- Cheng, Z., Wehrmeyer, J. A., and Pitz, R. W. (2003) "Downstream Interaction of Lean Premixed Flames," Proceedings of the Third Joint Meeting of the United States Sections of the Combustion Institute, Chicago, IL, March 16-19.
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- Frieden, D., and Sick, V. (2003a) "Investigation of the Fuel Injection, Mixing and Combustion Processes in an SIDI Engine using Quasi-3D LIF Imaging," SAE Technical Paper Series, 2003-01-0068
- Frieden, D., and Sick, V. (2003b) "A Two-Tracer Strategy for Quantitative Oxygen Imaging in Engines Applied to Study the Influence of Skip-Firing on In-Cylinder Oxygen Contents of an SIDI Engine," SAE Technical Paper Series, 2003-01-1114
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- Mosbacher, D. M., Wehrmeyer, J. A., Pitz, R. W., Sung, C.-J., and Byrd, J. L. (2002b) "Experimental and Numerical Investigation of Premixed Tubular Flames, Proceedings of the Combustion Institute, 29, pp. 1479-1486.
- Osborne R. J., Wehrmeyer, J. A., and Pitz, R. W. (2000) "A Comparison of UV Raman and Visible Raman Techniques for Measuring Non-Sooting Partially Premixed Hydrocarbon Flames," AIAA 38th Aerospace Sciences Meeting, Paper No. AIAA-2000-0776, Reno, Nevada, January 10-13.
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Students Graduated - University of Michigan

Boris Stojkovic, MSE in Mechanical Engineering, 2000, "Fuel Injector Characterization Using Simultaneous Planar Mie Scattering and LIF – Layout and Sources of Interference"

Doug Frieden, MSE in Mechanical Engineering, 2002, "Characterization of the Fuel Injection, Mixing and Combustion Processes in an SIDI Engine using Quantitative 2D and 3D Laser-Induced Fluorescence Imaging"

Boris Stojkovic, PhD in Mechanical Engineering, 2003, “Development and application of a time and space resolved optical diagnostic for soot temperature and concentration in a spark-ignited direct-injection engine”

Rui Zhang, PhD pre-candidate is working on fuel tracer issues related to the project and participated in some of the work

Udo Fissenewert, a PhD student from the Technical University of Berlin performed the NO measurements.

Undergraduate students involved in shorter-term research projects:

Mary Brett, 2000, Setup and installation of a Raman-shifting cell

Brian Miller, 2002, 3D flame propagation assessment in a SIDI engine

Students Graduated - Vanderbilt University

Zhongxian Cheng, MS in Mechanical Engineering, 2001, “Visible Laser Raman Diagnostics Application in Partially Premixed Flames of Premixed Fuel Versus Hot Products”

David Matthew Mosbacher, MS in Mechanical Engineering, 2002 “An Application of Non-Intrusive Laser-Based Diagnostics in Tubular Flames”

Zhongxian Cheng, PhD candidate, expected graduation May 2004, “Experimental and Numerical Investigation of Flame Structures for Stretched Lean Tubular/Planar Flames and Oxygen-Enhanced Flames”

Douglas A. Oguss, Undergraduate Senior Honor Thesis, April 1999, “Chemical Simulations for Laser and Flame Applications”