




## Propagation Characteristics of Hydrogen-Air Triple Flames Revealed by Direct Numerical Simulation

Hong G. Im and Jacqueline H. Chen have recently studied the structure and propagation characteristics of a triple flame formed in a hydrogen-air scalar mixing layer using direct numerical simulation with detailed chemical kinetics and transport models.

The triple flame is a canonical edge-flame structure that can potentially describe the flame stabilization mechanism at the base of a lifted turbulent jet diffusion flame. A triple flame is comprised of a curved premixed flame front spanning rich to lean compositions propagating along the stoichiometric mixture fraction line and a trailing diffusion flame formed from the excess fuel and oxidizer in the premixed branches. The propagation speed of the triple flame is different from that of the stoichiometric premixed flame and depends on various parameters including heat release, preferential diffusion, and mixture fraction gradient.

An analysis of direct numerical simulation data for a freely propagating hydrogen-air triple flame revealed that the enhancement of the propagation

speed is attributed mainly to flow divergence, and its value is proportional to the square root of the density ratio across the flame, consistent with earlier findings in the study of a methanol-air triple flame (see CRF News 19:2). It was also found that the three-branched structure of a hydrogen-air triple flame is best visualized by the reaction rate of H atom, one of the most important radical species in the hydrogen-air system.

Hong and Jackie have also investigated the effect of unsteady strain rate by imposing a pair of counter-rotating vortices onto a propagating triple flame. Figure 1 shows three sequential snapshots of the event during an interaction. It is found that, when the triple flame is subjected to intense strain rate induced by the vortices, the leading edge of the triple flame retreats backward, demonstrating the existence of negative displacement speed. The parametric quantification of the effect of strain on the stabilization speed is currently in progress. It is anticipated that the study will provide a valuable dataset to assess various computational submodels for partially premixed turbulent combustion. 

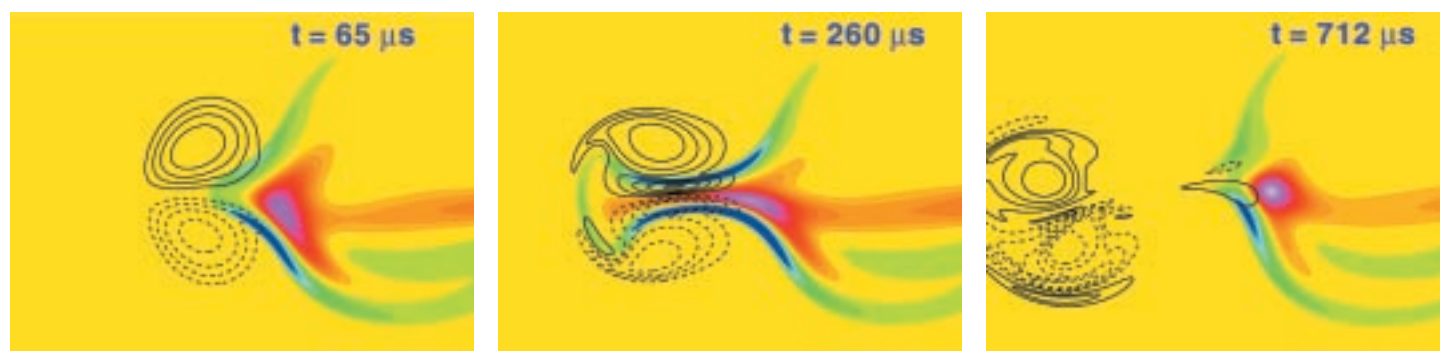


Figure 1. The time sequence of a hydrogen-air triple flame interacting with a pair of counter-rotating vortices reveals the effect of unsteady strain on flame propagation and structure. The color contours show the reaction rate of H atom; blue corresponds to H-atom consumption and purple to H-atom production. The line contours indicate the vorticity field, with the solid black line indicating clockwise rotation and the dashed line counterclockwise rotation. The H-atom reaction rate contours indicate that the three branches of the flame structure—the lean and rich premixed flames and the trailing diffusion flame—are all distorted by the vortices.



Eighty-four participants attended the Accelerated Strategic Computing Initiative (ASCI)/Academic Strategic Alliance Program DOE Lab Workshop on Turbulent Reacting Flow Simulation, which was hosted at the CRF on August 30-31, 1999. Jackie Chen and Professor Bill Reynolds of Stanford University developed a technically focused agenda, which included presentations from ASCI Alliance Universities (Stanford, Cal Tech, Chicago, Utah and Illinois) and Lawrence Livermore, Los Alamos, and Sandia National Laboratories as well as informal discussions and laboratory tours.

### **Biomass Conferees Visit CRF**

The CRF recently hosted 62 visiting researchers who were attending the Fourth Biomass Conference of the Americas, held in nearby Oakland CA. The CRF's Larry Baxter served on the Conference Program Committee and was an active participant in the conference proceedings. The visitors included scientists from 12 European countries and Japan, as well as many U.S. universities, industrial firms, national laboratories, and government agencies. They had the opportunity to visit 16 of the CRF labs, including many of the new CRF Phase II labs. In addition to the formal Conference, the CRF hosted the biannual meeting of the International Energy Agency's Biomass Combustion Working Group at the CRF.



Bob Carling describes the Alternative Fuel Diesel Engine Project to visitors during the recent Sandia Day VIP Tour. Shown here is the piston designed to provide optical access to the combustion process.



Dr. Jürgen Wolfrum (left) from the University of Heidelberg, Germany, visited the Combustion Research Facility to talk with staff and present a seminar titled "Laser Diagnostics in Combustion and Biology." He is shown with his host Frank Tully (right) and David Chandler.

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# EGR Mixing Measured in a Multicylinder Diesel Engine

In the high-speed, direct-injected diesel engine currently being developed for automotive applications by the Partnership for a New Generation of Vehicles, the use of exhaust-gas recirculation (EGR) will be a principal mechanism for controlling exhaust emission of  $\text{NO}_x$ . It is anticipated that large flowrates of EGR may be used under some conditions. Assuring uniform mixing, along with a balanced cylinder-to-cylinder distribution of this EGR, may be a serious challenge for the engine designer.

Bob Green is making measurements of EGR mixing in a Volkswagen 1.9L TDI — a small-bore, high-speed, four-cylinder, direct-injection diesel engine that is currently being sold for passenger vehicle applications. Optical access is obtained utilizing a specially designed spacer between the head and the intake and exhaust manifolds as illustrated in Figure 1. An optical path, created between the top and bottom windows in the spacer, provides access to the intake charge as it exits the manifold and enters the intake port. This allows Bob to determine the average concentration of EGR in the flow of fresh charge entering the intake port of each cylinder. The laser beam can also be moved across each window. By doing this Bob can measure a one-dimensional variation in the EGR concentration across each port.

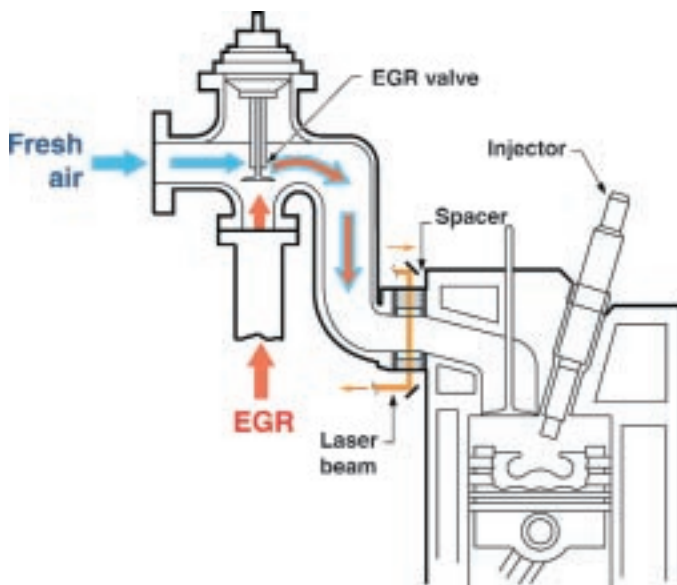


Figure 1. A schematic illustration of the application of infrared laser absorption to measure the concentration of EGR entering the engine cylinder.

The concentration of EGR entering the cylinders is measured using a diode laser tuned to an isolated  $\text{CO}_2$  absorption transition. The spectra obtained are fitted with a theoretical lineshape profile to give the average concentration of  $\text{CO}_2$  in the optical path.

It is anticipated that the primary EGR mixing problems, such as cylinder-to-cylinder maldistribution, are most likely to occur during transients in the engine operation rather than during steady-state conditions. Thus the data are resolved relative to the sequence of engine cycles that make up the engine transient, in addition to being resolved through the intake stroke of each cycle and ensemble-cycle averaged. The data in Figure 2 were

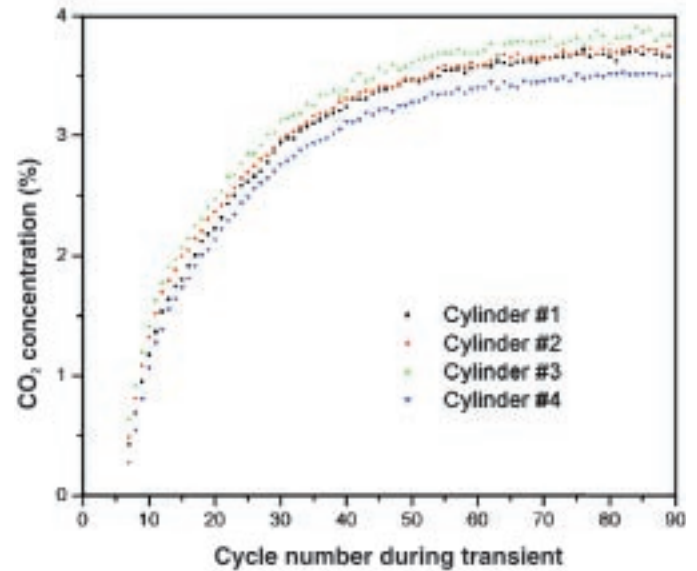



Figure 2. Measurements of the  $\text{CO}_2$  concentration in the intake flow of each cylinder during a step-change increase in the EGR flow occurring at cycle 0. Engine speed was 1500 rpm and accelerator position was 30%.

obtained during an engine transient where, at constant engine speed and load, EGR flow was rapidly activated to a high flowrate. These data illustrate the rise in concentration of EGR in the intake flow of each cylinder as a function of cycle number following the initiation of the EGR flow at cycle 0. Furthermore, these data suggest a small maldistribution of EGR between cylinders during the transient. 



## Transient Response of Premixed Flames Studied

Combustion systems rely on turbulence and large-scale flow unsteadiness to provide sufficient mixing and flame stabilization to ensure efficient and clean combustion. The resulting reacting flow involves significant interaction between unsteady flow dynamics and flame chemistry. The associated transient flame response dictates the incidence of extinction, reignition, and pocket formation. Adequate understanding and predictive modeling of these flows is necessary for advancing the state of the art, thereby improving combustion efficiency and reducing pollutant emissions from combustion devices.

Peter Wyckoff and Habib Najm, in collaboration with Omar Knio of the Johns Hopkins University, have developed algorithms and codes for computing two-dimensional, unsteady reacting flow with detailed chemical kinetics. Optimized operator-split stiff integration techniques have been developed and utilized to allow efficient modeling of hydrocarbon flames in laboratory scale flows on both shared and distributed memory parallel hardware. These codes have been used to study the dynamics of methane-air flames in unsteady vortical flows and to provide detailed chemical and flow comparisons with experimental measurements at the CRF.


One focus of these studies has been the interaction of a counter-rotating vortex pair with a premixed planar methane-air flame. This flow was investigated using a chemical mechanism with 32 species and 177 reactions. The transient response of the flame to the unsteady strain-rate disturbance induced by the vortex pair was studied under both stoichiometric and rich conditions.

Based on global flame time scale arguments, one would expect the thicker and slower-propagating rich flame to exhibit longer time scales, and hence slower time response. In fact, the present results exhibit the opposite behavior. The rich flame is found to respond faster by tending more quickly towards extinction. The observed difference in peak heat release rate time history on the vortex-pair centerline flame segment is shown in Figure 1. This observed faster response at rich conditions is also supported by experimental

measurements of Phillip Paul at the CRF on a vortex-pair interaction with a premixed methane-air V-flame.

Numerical results suggest that this faster response of the rich flame may be related to the enhanced role of H atom and the reduced role of OH radical at rich conditions. Moreover, it is not unreasonable to expect that the rich flame would extinguish faster than the stoichiometric flame under similar tangential strain-rate time histories.

More generally, these findings suggest that the chemical response of internal flame structure due to strain-rate disturbances is not governed by the global flame time scale based on the burning speed and flame thickness, but rather by other time scales pertaining to the reaction-diffusion processes of relevant radicals internal to the flame.

Current activities are focused on further investigations of transient flame response characteristics, employing other chemical mechanisms and flow-flame conditions, as well as extensive comparisons with experiments. 

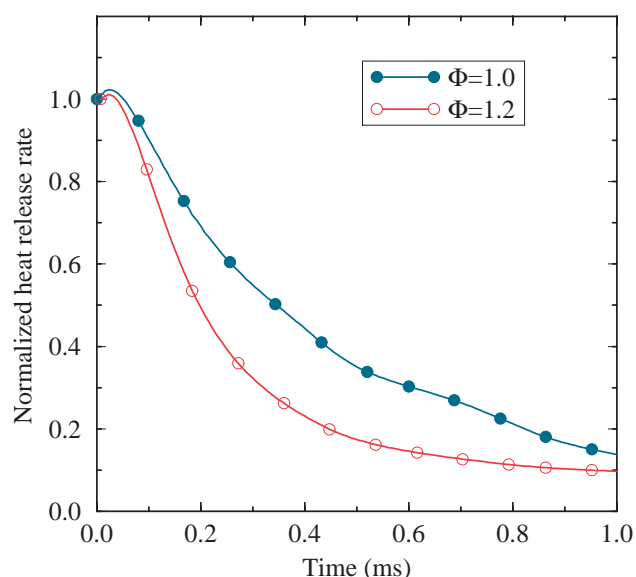


Figure 1. Time evolution of peak heat release rate in the flame centerline segment for stoichiometric and rich flame conditions. Faster response time is observed in the rich flame, in agreement with experimental measurements.



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