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Unexpected effects of preferential transport in turbulent premixed flames

When considering the structure of turbulent premixed flames, it is normally taken for granted that the equivalence ratio (ER) ϕ is the same on the reactant and product sides of the flame, even if preferential diffusion causes deviation inside the flame. However, multiscale measurements in methane-air flames stabilized on a bluff body burner from Cambridge University (see companion article at right) have revealed that the basic assumption that mean atom balances and stoichiometry are conserved across a turbulent premixed flame does not always hold true.

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Continuing collaborations on stratified combustion

Stratified combustion, in which the flame propagates through a non-uniform fuel-air mixture, is common in a wide range of practical devices. However, relatively little is known about the fundamental effects of stratification on turbulent flame structure or the accuracy of current combustion models in predicting stratified flames. Sandia has been collaborating with the University of Cambridge, UK, and the Technical University of Darmstadt, Germany, to improve our fundamental understanding of stratified turbulent flames and provide detailed data



Figure 1-1. Photographs of two highly stratified flames stabilized on the Cambridge burner: (a) nonswirling and (b) swirling. The white line in (a) indicates the region where the flame is burning through the middle of the turbulent mixing layer between two annular streams of different equivalence ratio ($\phi_{inner} = 1.125$, $\phi_{outer} = 0.375$).

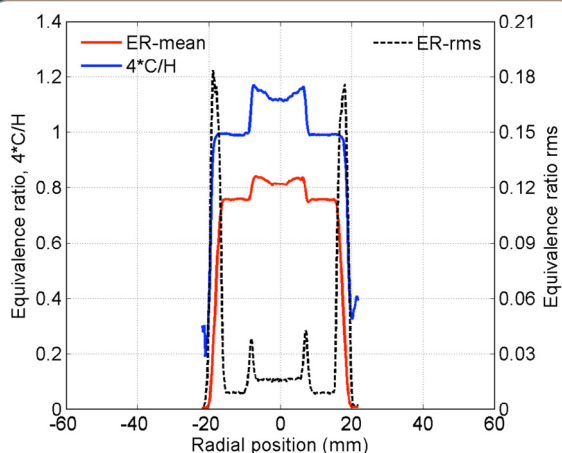


Figure 2-1. Radial profiles of measured equivalence ratio ϕ (mean and rms) and C/H atom ratio (mean) in a non-swirling premixed flame at axial location $z = 10$ mm. The conical flame is 7–8 mm from the burner centerline with combustion products on the inside.

sets for model validation. Selected cases from the Darmstadt stratified burner have already been used as targets for model comparisons at the TNF10 Workshop (Beijing, July 2010). Velocity and scalar measurements obtained in Germany have been complemented by temperature, OH LIF, and acetone LIF imaging experiments carried out in Jonathan Frank's Advanced Imaging Laboratory with visitor Benjamin Böhm.

Rob Barlow, Matt Dunn, and Bob Harmon from the CRF have been working with Mark Sweeney and Simone Hochgreb of Cambridge to investigate a second stratified turbulent

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burner. This burner borrows from the co-annular design developed by TU Darmstadt but increases complexity of the flow field by using a central bluff body rather than a pilot for flame stabilization and by including variable swirl in the outer annular flow. The theme of offering modeling targets with progressively increasing complexity, as well as parametric variation on each burner, is central to the TNF Workshop process.

Twelve turbulent methane–air flames were investigated on the Cambridge burner, with varying stratification ratio ($SR = \phi_{\text{inner}}/\phi_{\text{outer}} = 1.0, 2.0, 3.0$) between the two annular flows and varying swirl number (0 to approximately 0.7) in the outer annulus. All cases had bulk velocities of 7.5 m/s in the inner annulus, 15 m/s in the outer annulus, and 0.4 m/s in the coflow. The Figure 1-1 photographs show two cases with stratification ratio 3 ($\phi_{\text{inner}} = 1.125, \phi_{\text{outer}} = 0.375$), a non-swirling flame on the left and a swirling flame on the right. The most interesting region of each stratified flame is where the center of the turbulent flame brush crosses the center of the mixing layer (mean ϕ halfway between values in the two annular streams) because this is where the flame is affected by the largest gradients in equivalence ratio. For the case shown in Figure 1-1(a), this mean crossing occurs near 50 mm downstream of the bluff body and 14 mm from the burner centerline, as indicated in the figure. The instantaneous radial gradient of ϕ at this location can exceed 0.3 mm^{-1} , which is more than enough to cause important changes in the structure of a propagating laminar flame.

The Raman/Rayleigh/CO-LIF laser diagnostic system in the Turbulent Combustion Lab at the CRF achieves 0.1 mm resolution in line-imaged measurements of temperature, all major species ($\text{N}_2, \text{O}_2, \text{CH}_2, \text{CO}_2, \text{H}_2\text{O}, \text{CO}, \text{H}_2$) and local

equivalence ratio ϕ with precision sufficient to determine scalar gradients within the instantaneous internal flame structure. Crossed-planar imaging of OH fluorescence was applied to measure the instantaneous 3D flame normal where the flame intersects the multiscale line segment. This information has been used to determine the 3D gradient of temperature and reaction progress variable as well as to obtain statistics on flame surface density and curvature. Complementary velocity measurements using particle image velocimetry (PIV) are being conducted at Cambridge.

In stratified flames the progress variable c depends on the local equivalence ratio, such that $c = (T - T_u)/(T_b(\phi) - T_u)$, where T_u is the unburnt reactant temperature, and T_b the adiabatic equilibrium burnt gas temperature. Dissipation of the reaction progress variable, $\chi_c = \alpha \nabla c \cdot \nabla c$, is an important term in some premixed and stratified combustion modeling approaches. Local ϕ and the gradient of c must be measured in order to determine this scalar dissipation term in a stratified flame. The measured gradient in c is also used to determine flame surface density, another important quantity in models for premixed and stratified flames.

Figure 1-2 below includes example scalar and velocity results from the flame and measurement location shown in Figure 1-1(a). The velocity measurements show the extent of the recirculation zone and also demonstrate that the scalar probe volume (6-mm extent) crosses the shear layer between inner and outer annular streams. The results for ∇c and χ_c indicate that stratified flames tend to be thicker than homogeneous premixed flames at the same equivalence ratio. Analysis of the complete data set is in progress, and it is hoped that these flames will be useful targets for future model comparisons.

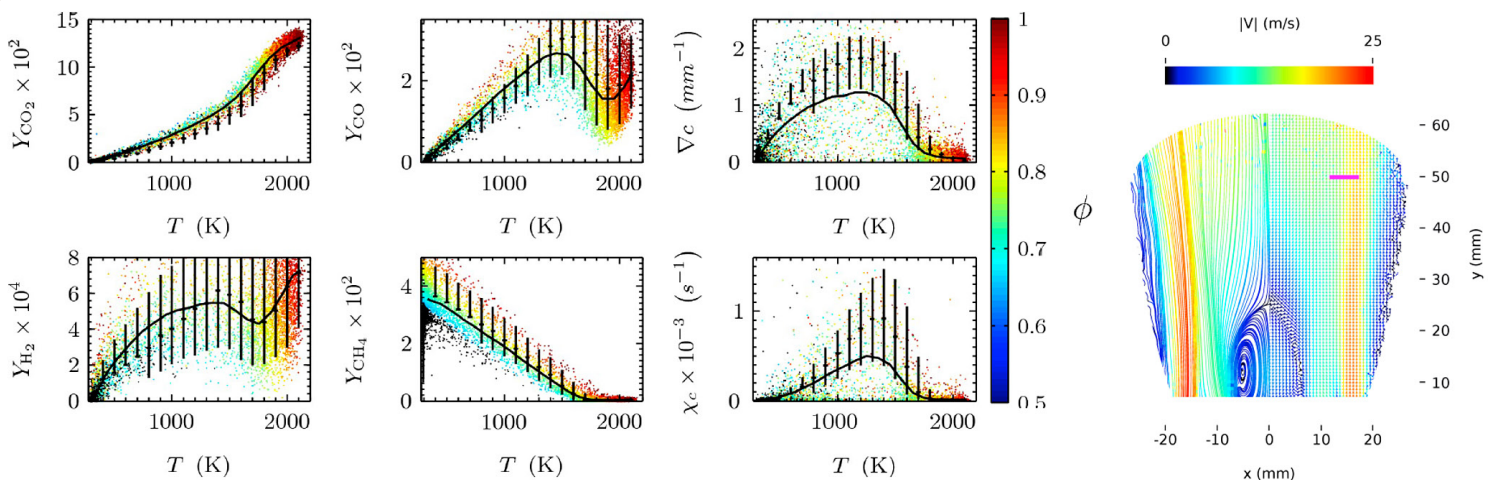


Figure 1-2. Scalar and velocity results from the same measurement location as in Figure 1-1. Scatter data are color coded according to the local equivalence ratio. The black curves show conditional means of the scatter data. The crosses show the range of results (maximum, mean, minimum) corresponding laminar premixed flame calculations evaluated at the locally measured values of equivalence ratio and progress variable. The velocity field from preliminary PIV measurements is plotted as interpolated streamlines on the left and directional arrows on the right, each color coded by velocity magnitude in the measurement plane.

Welcome to the CRF Celebration

NOVEMBER EIGHTH TWO THOUSAND TEN



CRF opens its doors to inaugurate the new General Access Area

On Monday, November 8, the CRF invited staff members and their families—including many excited children—to an Open House commemorating the launch of the General Access Area (GAA) and the new Greenville Road entrance. For the first time, people who have not been cleared ahead of time can drive (or bike!) directly onsite.

Bob Carling, director of the Transportation Energy Center, gave a short welcoming address thanking the many important team members who worked tirelessly to bring about the GAA. He then briefly outlined the history of the CRF and its changing role in combustion research as times have changed.

“Thirty years ago the seminal event [in the creation of the CRF] in the early ’70s was the oil embargo, and bringing together lasers to interrogate combustion systems in a new and different way,” he said. “The seminal event of today is the open campus. I think we’ll mark this time as a real change for this laboratory, particularly the CRF, to accelerate innovation and have more impact with our customers and stakeholders than ever before.”



If the challenge for the first 30 years was the *what*: using lasers to interrogate combustion, today it’s the *how*: how do we work together in a new and different way with our customers? “That is how we as a laboratory can have more impact out in the future,” Bob noted before inviting guests to tour the facilities (including a sneak peek at the new research building that will officially open in January).



In the first month since the opening of the GAA, over 200 visitors have been badged into the CRF.

Top: Director Bob Carling addresses the visitors CRF visitors on November 8. Right: Friends and family of CRF staff tour the open collaboration spaces of the new CRCV building. Left: two of the smallest visitors make use of the new CRCV collaborative meeting space while delving into their gift bags, which contained a solar calculator, a Sandia mouse pad, a star-shaped magic marker, color-changing pencils, and several other science-based items. (Photos by Daniel Strong)

Visit from SINTEF Energy Research promotes collaboration

On October 15, six managers and staff from SINTEF Energy Research in Norway visited the CRF to plan research collaborations within the scope of a Memorandum of Understanding between Sandia and SINTEF that was signed a year ago. The visit was among the first to be facilitated by the streamlined administrative procedures made possible by the opening of the GAA, which includes the CRF complex.

Sandia and SINTEF are engaged in longstanding collaborative research efforts focused on the development and experimental validation of turbulent combustion models targeting environmentally benign energy-conversion technologies. Broadening of this collaboration, including possible initiatives related to biofuels, internal combustion engines, and combustion processes compatible with carbon capture and sequestration, was discussed during the visit.

At right: John Dec and visiting SINTEF researcher Marie Bysveen tour the HCCI Engine Combustion Fundamentals Lab. (Photo by Karen McWilliams)

Unexpected effects of preferential transport *(Continued from page 1)*

In the Cambridge burner the flame is stabilized by a central bluff body (12.7-mm diameter) and the resultant recirculation zone of combustion products. Figure 2-1 (page 1) shows radial profiles of equivalence ratio and the carbon-to-hydrogen atom ratio (calculated from the measured major species: N_2 , O_2 , CH_4 , CO_2 , H_2O , CO , and H_2) taken 10 mm downstream of the bluff body surface. At this upstream location, the flame bush is quite thin—only a couple of millimeters—yet the measured equivalence ratio increases by nearly 10% and the C/H ratio increases by more than 15% going through the nearly vertical flame brush from reactants to products.

These unexpected results cannot be attributed to experimental error. In fact, measurements across the lean premixed laminar flame shown in Figure 2-2 are in very good agreement with a Chemkin calculation of an unstrained flame, using GRI Mech 3.0 and multi-component transport.

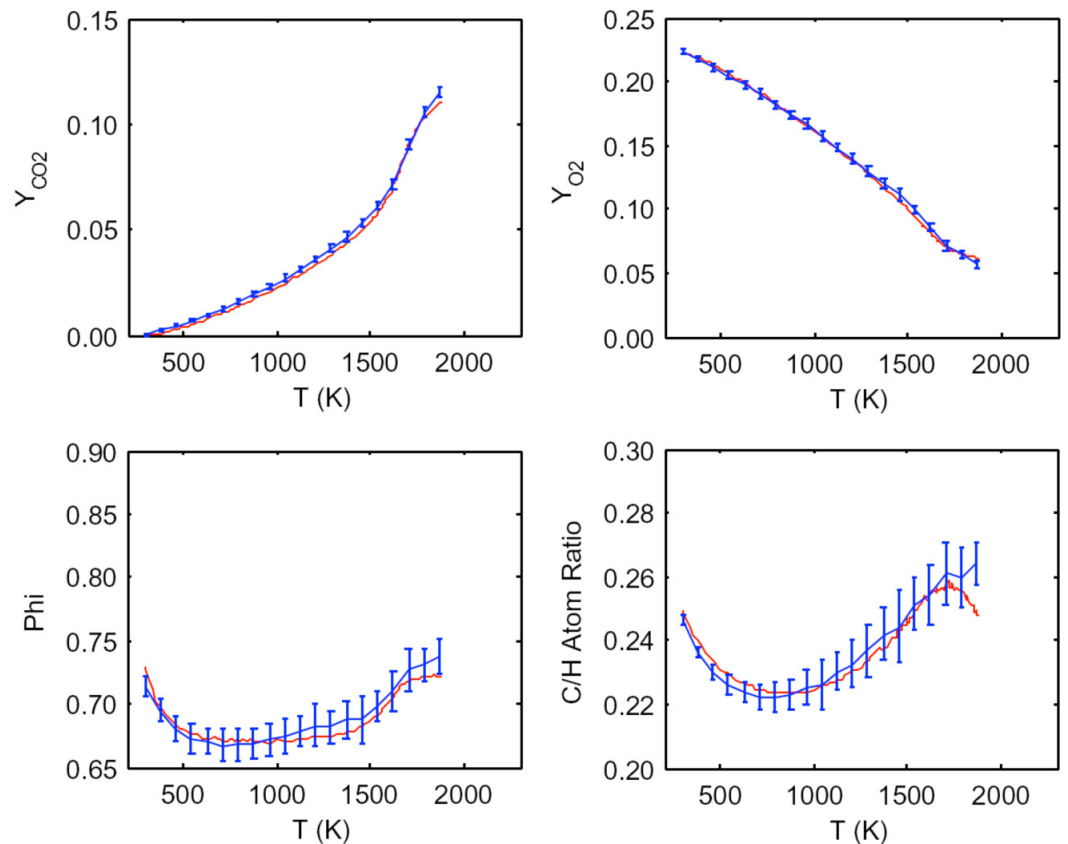
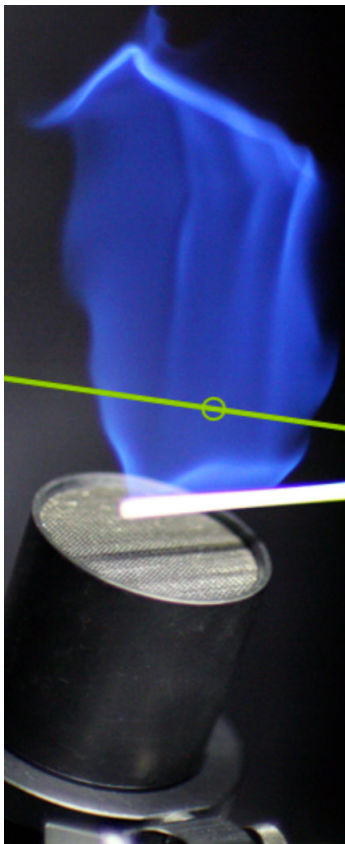


Figure 2-2. Photograph of a laminar “vertical” premixed flame at $\phi = 0.73$, and comparisons of measured and calculated results for selected mass fractions, the equivalence ratio (Φ), and the C/H atom ratio plotted vs. temperature.

The corresponding plots of scalars vs. temperature are shown in Figure 2-3 for a lean premixed turbulent flame stabilized on the Cambridge burner. Along with the deviation of the conditional mean results for ϕ and C/H in the turbulent flame from those of the laminar calculation, there are significant deviations for the mass fractions of CO_2 and O_2 , such that CO_2 is higher than expected in the burnt products and O_2 is lower. Effects on the mass fractions of other species are less obvious. Similar behavior is observed in the near-field results for all the Cambridge burner flames.

The observed variation in ϕ and the C/H ratio are believed to be the result of differential molecular diffusion, which is known to alter the local structure of curved premixed flames (both laminar and turbulent) by focusing or defocusing fast-diffusing species. As far as we know, differential diffusion has not been shown to cause changes in mean composition and stoichiometry going from reactants to products across a turbulent premixed flame.

It was first hypothesized that depletion of the C/H ratio was driven by preferential diffusion of molecular hydrogen through the preheat zone, followed by turbulent mixing and downstream advection away from the local flame brush. However, as

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Unexpected effects of preferential transport in turbulent premixed flames (Continued from page 4)

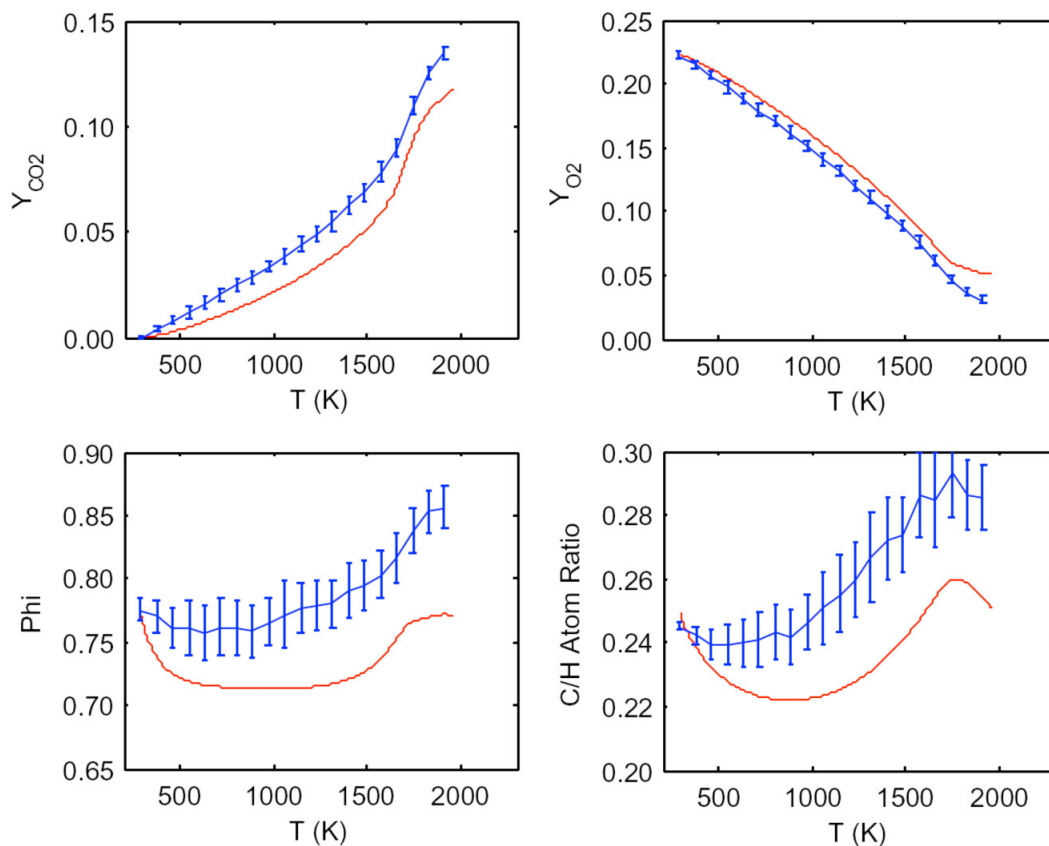


Figure 2-3. Photograph of premixed turbulent flame SwB2 and comparisons of measured results and laminar unstrained 1D Chemkin calculations at $\phi = 0.77$.

suggested by Forman Williams in discussions at the TNF10 Workshop, preferential transport of H_2O ahead of CO_2 probably also contributes to the increase in C/H ratio. Figure 2-4 shows spatial profiles of the mole fraction ratios $X_{\text{H}_2\text{O}}/X_{\text{CO}_2}$ and $(X_{\text{H}_2} + X_{\text{H}_2\text{O}})/X_{\text{CO}_2}$ from an unstrained premixed laminar flame calculation, illustrating preferential diffusion of H_2 and H_2O through the preheat zone ahead of CO_2 .

Matt Dunn and Rob Barlow of the Reacting Flow Research department conducted subsequent experiments on several simple laminar and turbulent premixed burners to better understand the contributing physical mechanisms. This work indicates that the presence of the recirculation zone is a key factor in amplifying the effects of preferential transport. The magnitude of the effect on the C/H atom ratio, measured in a premixed bluff-body burner, increased with increasing Reynolds number. Notably, Ed Richardson (former CRF postdoc, now at University of Southampton, UK) suggested very early in this work that conditions in the recirculation zone were likely to contribute to the observed effects.

At present, it is not known whether this preferential transport phenomenon will prove important for accurate modeling of premixed (and stratified) turbulent flames. However, current information suggests that similar effects may be present in any premixed hydrocarbon flame that is stabilized by a strong recirculation zone.

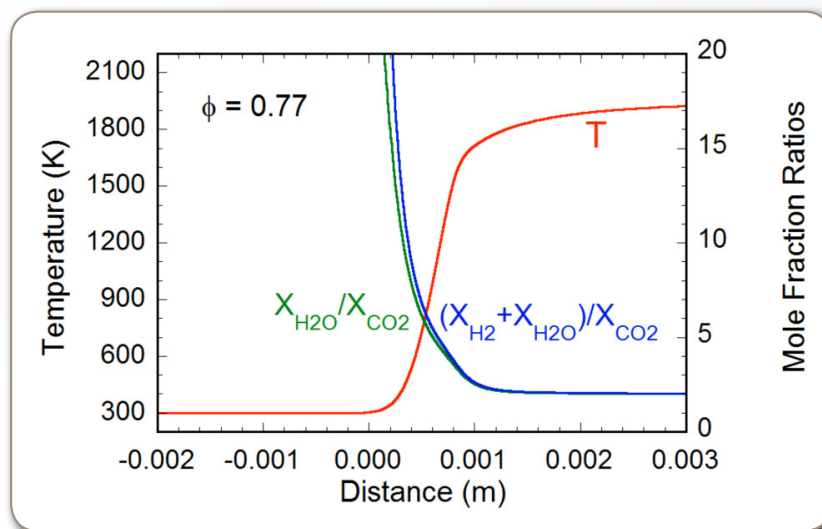


Figure 2-4. Spatial profiles of the mole fraction ratios $X_{\text{H}_2\text{O}}/X_{\text{CO}_2}$ and $(X_{\text{H}_2} + X_{\text{H}_2\text{O}})/X_{\text{CO}_2}$ from an unstrained premixed laminar flame calculation at $\phi = 0.77$ (Chemkin with GRI 3.0 and multicomponent transport) illustrating preferential diffusion of H_2 and H_2O ahead of CO_2 .

Green Engineering Academy students visit the CRF

As Kermit the Frog once lamented, it's not easy being green. Students in the inaugural class of Livermore High School's Green Engineering Academy are getting some help in living up to the connotations of that color—once synonymous with money, but now representing the environmental movement—through a partnership with Sandia. On January 4, the Academy students and their teachers toured the CRF and met the Sandia mentors who will guide their research. The LHS Green Engineering Academy is a “school within a school” focused on green technology and engineering.

Deputy Director Andy McIlroy welcomed the students to the CRF and explained some of the areas of research. “Our work in the energy field spans a wide area and has a lot of impact,” he says. “The work that we do here in the CRF helped get you here today, quite literally.” In small groups, the students rotated through the Hydrogen Combustion Lab, hosted by Victor Salazar; Flame Diagnostics and Chemistry Lab, hosted by Nils Hansen and Scott Skeen; Turbulent Combustion Lab, hosted by Isaac Ekoto and Adam Ruggles; Heavy Duty Diesel Lab, hosted by Mark Musculus; and the Alternative Fuels Engine Lab, hosted by Chuck Mueller.



Mark Musculus shows students Areli Hernandez, Laila Hassen, Laurena Landavazzo, and Chris Ingwerson a frame of a high-speed movie of combustion luminosity taken through the transparent piston of an optical diesel engine. (Photo by Randy Wong)



“The tour was pretty amazing,” said LHS student Ben Davidson. “It’s really interesting, all the cool stuff they do with alternative energy and hydrogen. I learned about the intricate ways that the researchers view what happens inside an internal combustion engine.”

Academy teacher Mike Waltz says that in addition to seeing interesting labs and equipment, the tour enabled the students to see what scientists really do day to day. “I guess you’d call it career familiarization,” he says. “They hear about different jobs in science and engineering, but it’s much different to actually see where people work and the equipment they use.”

Green Engineering Academy students Laila Hassen, Areli Hernandez, and Laurena Landavazzo take a close look at the burner and optics table in the Turbulent Combustion Lab. (Photo by Randy Wong)



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