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Probing transient flow-flame interactions:

Effects of nitric oxide and water vapor on the dynamics of extinction and re-ignition

In turbulent flames, intermittent fluctuations in transport rates can lead to localized extinction followed by re-ignition. These events are particularly challenging to model because of the complex interactions between transient flows and flame chemistry. Combined experimental and numerical studies of isolated vortex-flame interactions in a counterflow provide detailed insight into the dynamics of extinction and re-ignition in transient flows. An ongoing series of studies couples imaging diagnostics and direct numerical simulations (DNS) to better understand the effects of additives on extinction and re-ignition for a wide range of fuels. The initial phase of this investigation focused on hydrogen combustion because it provides a simple chemical system for investigating these interactions, and it is an important submechanism of hydrocarbon chemistry that controls high temperature radical branching and thermal explosion in high pressure, intermediate temperature conditions. Practical applications of hydrogen combustion have received renewed interest as a result of recent increases in fossil fuel costs and concerns about climate change.

During an extended visit to Sandia, Uendo Lee (Korea Advanced Institute of Science and Technology) worked with CRF researchers Jonathan Frank, Sebastian Kaiser, Chun Sang Yoo, and Jackie Chen to study the

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Improving low-load combustion in HCCI engines

Homogeneous charge compression ignition (HCCI) is an alternative piston-engine combustion process that can provide both high efficiency and very low emissions of nitric oxides (NO_x) and particulates. Several technical hurdles must be overcome, however, before this promising technology becomes viable. One of the most important hurdles is to improve combustion efficiency at low loads and reduce the associated emissions of carbon monoxide (CO) and unburned hydrocarbons (HC).

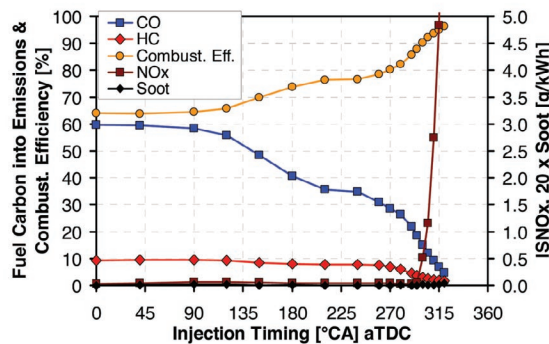


Figure 1. The effect of injection-timing retard on emissions and combustion efficiency for an idle fueling of $\phi = 0.12$, hollow-cone injector, 120 bar injection pressure. Note that 0°CA is taken to be TDC of the intake stroke and 360°CA is TDC of the compression stroke.

Previous work (see *CRF News* March/April 2003) has shown that this problem occurs because combustion temperatures become so low with the very dilute fuel/air mixtures used for low-load HCCI ($0.1 \leq \phi \leq 0.2$) that combustion does not go to completion before being quenched by the expansion stroke. This previous work also showed that strati-

fying the fuel/air mixture could improve low-load combustion efficiency by concentrating the fuel in the central part of the combustion chamber, so the mixture is locally less dilute. However, the amount of stratification allowable is limited because eventually the concentration of fuel in the richest regions increases to the point that combustion temperatures are sufficient to produce NO_x emissions. In this previous work, combustion efficiency

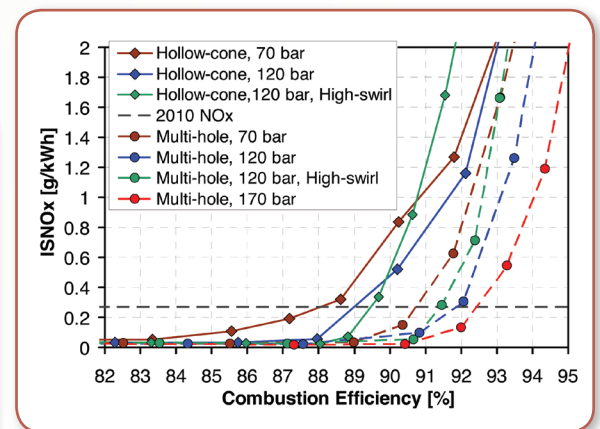


Figure 2. Tradeoff between combustion-efficiency and NO_x emissions for various injectors, injection pressures and swirl, $\phi = 0.12$.

was increased from 51% for a well-mixed charge to 78% at the NO_x limit. Although this is a substantial improvement, it is still an unacceptably low combustion efficiency.

To address this problem, CRF researchers Wontae Hwang, John Dec, and Magnus Sjöberg conducted an investigation of various fuel-stratification techniques to determine which parameters are effective for improving the combustion-efficiency/ NO_x

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Improving low-load combustion in HCCI engines (continued)

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tradeoff. Performance and emissions measurements were made in an all-metal engine, and planar laser-induced fluorescence (PLIF) measurements of the fuel distributions were made in a matching optically accessible engine. Parameters examined included the type of fuel injector, the injection pressure, and the amount of in-cylinder air swirl. All data were acquired at a low-load condition corresponding to an idle fueling rate. The fuel was iso-octane, which has been shown to be a good surrogate for gasoline.

ciency improved with increased injection pressure, reaching a value of about 92.5% for the multi-hole injector with 170 bar injection pressure.

To better understand the differences in mixture formation for various mixture-formation parameters, an improved quantitative fuel-PLIF imaging technique was developed and applied. Typically, equivalence-ratio (ϕ) images of fuel distributions are produced by simply applying a calibration to PLIF images obtained using a fluorescent tracer in the fuel. This method, however, neglects the effect of temperature variations associated with the non-uniform fuel distribution. These variations occur because regions of higher fuel concentration experience greater evaporative cooling and reduced compression heating (due to the increased specific heat when more fuel is present). To overcome this problem, the temperature sensitivity of

the PLIF signal was mapped out at engine conditions, and an iterative technique was developed to correct the PLIF images for these thermal effects. As illustrated by the difference between the images in Figures 3a and 3b, this correction has a significant impact on the apparent fuel distribution. The correction technique also provides the corresponding temperature map, as shown in Figure 3c.

Figure 4 presents sequences of temperature-corrected quantitative “ ϕ -map” images for the hollow-cone and multi-hole

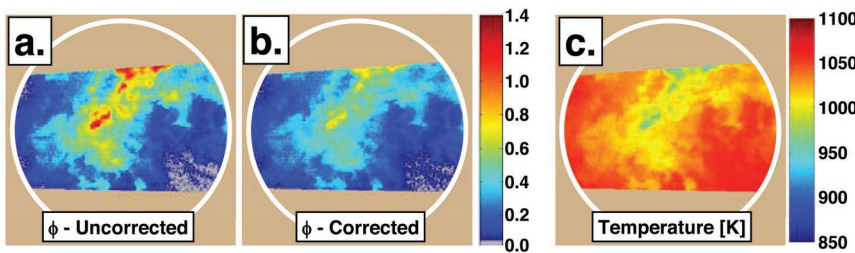


Figure 3. Fuel/air equivalence ratio (ϕ) images derived from a fuel PLIF image. Figure 3a is uncorrected and Figure 3b is corrected for the temperature variation associated with fuel stratification. Figure 3c shows the corresponding temperature field.

The required stratification was accomplished by decreasing the mixing time by using a gasoline-type direct fuel injector and progressively delaying the start of injection from early in the intake stroke until well up the compression stroke. An example of the changes in combustion efficiency and emissions with increasing stratification is shown in Figure 1. As can be seen, for a well-mixed charge (early injection timing), combustion efficiency is low and CO and HC emissions are high. However, as the fuel/air charge becomes progressively stratified with delayed injection, the CO and HC emissions fall substantially with a commensurate increase in combustion efficiency. This trend continues even for very late injection timings, but beginning at about 300°CA (for this case), NO_x emissions begin to rise rapidly. With this hollow-cone spray injector, using 120 bar injection pressure, a combustion efficiency of 89% could be achieved at the US-2010 NO_x emission standard, as shown in Figure 2. Although this efficiency represents a substantial improvement from the 2003 data, resulting mainly from a wider-angle hollow-cone spray, even higher efficiencies are desirable.

The results in Figure 2 also show that the multi-hole injector further improved the combustion-efficiency/NO_x tradeoff, increasing combustion efficiency at the US-2010 NO_x limit to 91.7% for the same 120 bar injection pressure. For both injectors, the NO_x-limited combustion effi-

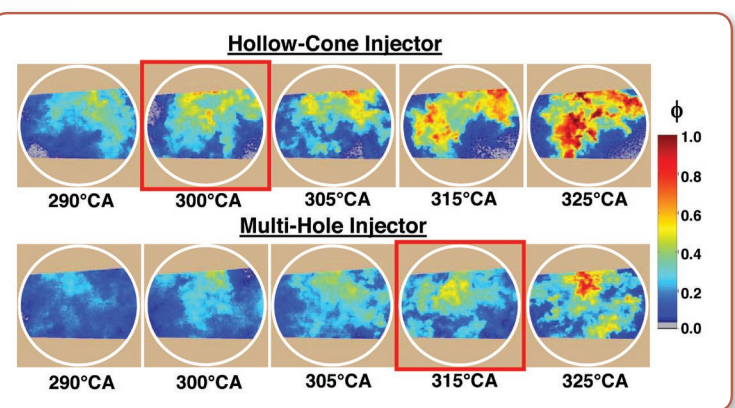


Figure 4. Series of ϕ -maps of the fuel distribution as injection is delayed for the hollow-cone and multi-hole injectors with 120 bar injection pressure. The red box around the 300°CA (hollow-cone) and 315°CA (multi-hole) images indicates that they correspond to the knee in the NO_x curves in Figures 1 and 2. The images were acquired at 365°CA in the mid-plane of the combustion chamber.

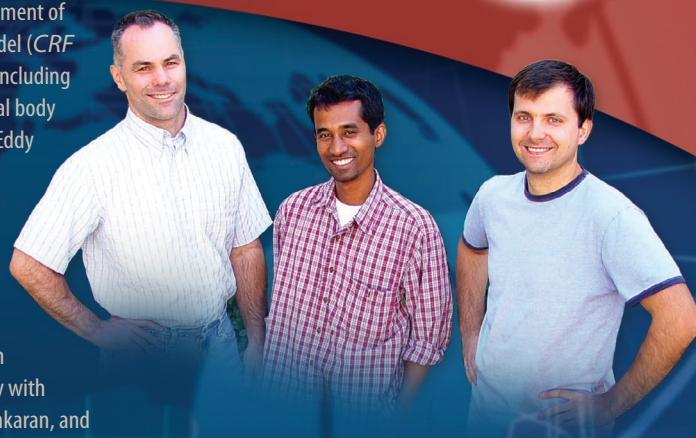
injectors. The sequences show how the delayed injection affects the fuel distributions present at the time of combustion (365°CA). For both injectors, the amount of mixture strati-

COMBUSTION RESEARCH FACILITY VISITOR PROGRAM



Vaidyanathan (Vaidya) Sankaran completed a postdoc working with Joe Oefelein in the area of Large Eddy Simulation. He started at the CRF in February 2006 and recently accepted a permanent position at United Technologies Research Center in East Hartford, CT. Vaidya played a major role in the development of advanced simulations techniques for turbulent combustion, with emphasis on the Linear Eddy Model (CRF News article May/June 2008). He collaborated extensively with researchers throughout the CRF, including Alan Kerstein, Rob Barlow, Jackson Mayo and Tomasz Drozda, and recently published a foundational body of work entitled "A Tabulated Closure for Turbulent Nonpremixed Combustion Based on the Linear Eddy Model" as part of the 32nd International Symposium on Combustion.

Tomasz (Tom) Drozda completed a postdoc working with Joe Oefelein in the area of Large Eddy Simulation. He started at the CRF in September 2005 and recently accepted a permanent position at Rolls Royce Aircraft Engines in Indianapolis, IN. Tom played a major role in the development of both advanced combustion models and high-pressure direct injection models, with emphasis on both fundamental laboratory flames and internal combustion engines. He collaborated extensively with researchers throughout the CRF, including Alan Kerstein, Rob Barlow, Jackson Mayo and Vaidya Sankaran, and contributed to many publications. His most recent is a publication accepted by *Combustion and Flame* entitled "Scalar Filtered Mass Density Functions in Nonpremixed Turbulent Jet Flames" (Vol. 155, 54-69, 2008).



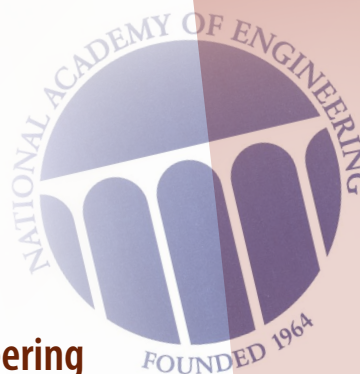
From left to right: Joe Oefelein, Vaidyanathan (Vaidya) Sankaran, Tomasz (Tom) Drozda.



Jim Miller inducted into the National Academy of Engineering

Jim Miller was inducted into the National Academy of Engineering on October 5. Jim was recognized for his "research on the theory and modeling of combustion chemistry that has led to universally applied codes for combustion modeling." Gary Grest, a Sandia staff member in Albuquerque, was elected at the same time.

Jim received his doctorate from Cornell University in 1974 and has worked at Sandia since that time. He was part of the founding staff of the Combustion Research Facility in 1980 and has had the title "Distinguished Member of the Technical Staff" since 1989. His research interests are principally in combustion chemistry and theoretical chemical kinetics. He is a Fellow of the American Physical Society, a Fellow of the American Association for the Advancement of Science, and a member of the American Chemical Society and The Combustion Institute, from whom he received the Silver Medal in 1990 and the Lewis Gold Medal in 2006. Jim currently serves as an associate editor of *Combustion and Flame* and is on the editorial advisory boards of *The Journal of Physical Chemistry* and *Theoretical Chemistry Accounts*. A special issue of *The Journal of Physical Chemistry A* (May 17, 2007) was devoted to a James A. Miller Festschrift in celebration of his 60th birthday.



James A. Miller
has been duly elected a Member of
the National Academy of Engineering of
the United States of America



and the same to be attested by the officers this
day of October in the year of

James Mark Jacobs
Chair

Thomas F. Beal
Home Secretary

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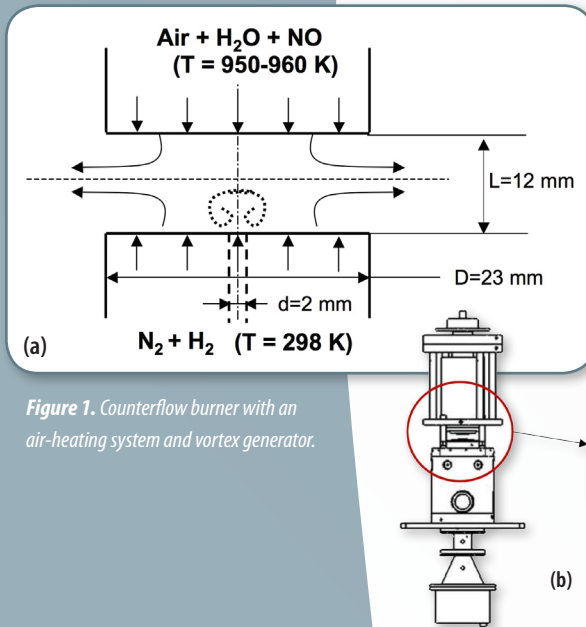


Figure 1. Counterflow burner with an air-heating system and vortex generator.

effects of nitric oxide (NO) and water vapor (H_2O) on the dynamics of extinction and re-ignition of a vortex-perturbed hydrogen diffusion flame in a heated counterflow configuration. Although the basic mechanisms by which NO and H_2O affect the ignition process are well-established, it is important to improve our understanding of the effects of these additives on the dynamics of extinction and re-ignition during transient flow-flame interactions.

Figures 1a-b show the axisymmetric counterflow burner configuration with heated air and nitrogen-diluted hydrogen issuing from the upper and lower ducts, respectively. Localized extinction was induced by impulsively driving a fuel-side vortex into a steady laminar counterflow flame.

The temporal evolution of the extinction and recovery of the flame was measured with OH planar laser-induced fluorescence (PLIF).

Direct numerical simulations of the experiments were used to analyze the chemical effects of H_2O and NO addition. The DNS was performed with Sandia's S3D code using a detailed $H_2/O_2/NO_x$ kinetic mechanism from Professor Fred Dryer of Princeton University.

The sequence of OH PLIF images in Figure 2a shows the deformation and localized extinction of the counterflow flame that was induced by the impinging vortex. The presence of OH indicates an intact system of high-temperature combustion chemistry, and the gap in the OH

layer identifies the extinguished region. In this experiment, the air stream was heated to a few degrees above the autoignition temperature of the steady counterflow mixtures. The flame re-ignited by inward propagation of an annular edge-flame.

Figure 2b shows that the addition of NO significantly alters the flame recovery dynamics by enabling the formation of an ignition kernel near the burner axis. The combination of annular edge-flame propagation and expansion of the ignition kernel accelerates the flame recovery. The addition of NO has a catalytic effect on the ignition of both hydrogen and hydrocarbon fuels, resulting in decreased autoignition temperatures. For hydrogen, the addition of NO alters the ignition process by turning the chain terminating steps related to HO_2 formation ($H + O_2 + M \rightleftharpoons HO_2 + M$) into chain-propagating steps related to OH formation ($NO + HO_2 \rightleftharpoons NO_2 + OH$, $NO_2 + H \rightleftharpoons NO + OH$).

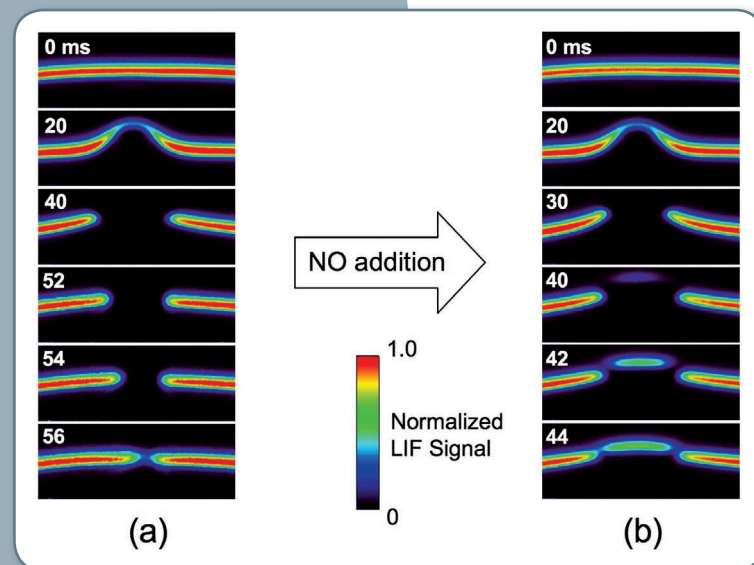


Figure 2. Sequence of OH LIF measurements shows the evolution of the flame-vortex interaction without NO doping (a) and with 160 ppm of NO added to the air flow (b). The air flow is heated to $T_{air} = 951$ K, and the fuel flow is N_2 -diluted hydrogen, with $X_{H_2} = 0.13$, $T_{fuel} = 298$ K.

The formation of an ignition kernel was also observed without NO doping when the temperature of the preheated air was increased to 960 K, as shown in Figure 3a. However, the flame recovered entirely by expansion of the ignition kernel while the annular edge flame receded until it extinguished. Figure 3b again shows that doping with NO produces the combined recovery mode.

Figure 3c shows that the addition of 1.2% water vapor (by volume) to the heated air delays the formation of the ignition kernel until after the annular edge flame is completely extinguished, thereby significantly increasing the total recovery time. The addition of water vapor to a reactant mixture lowers the reaction zone temperature, making the flame easier to extinguish and more difficult to ignite.

Figure 3d shows the flame response with the addition of both H_2O and NO. Due to the combination of the NO catalytic effect and the H_2O inhibiting effect, the induction time for the autoignition is between the H_2O addition case (Figure 3c) and the NO doping case (Figure 3b). The total recovery time is closer to that of the NO doping case because the catalytic effect of NO dominates over the inhibiting effect of water.

Direct numerical simulations of the experiments were performed to further elucidate the effects of NO and H_2O additives on extinction and re-ignition dynamics. Four different cases were considered: no additives (Case 1), doping with NO (Case 2), doping with H_2O and NO (Case 3), and doping with H_2O , NO, and Ar (Case 4). The fourth case isolates the chemical effect of water vapor addition from the thermal effect that results from the larger specific heat of H_2O . The addition of argon offsets the thermal effect of water, such that Case 4 has the same flame location and maximum flame temperature as Case 2.

(Continued on page 5)

Effects of nitric oxide (continued)

(Continued from page 4)

Simulations of the vortex-flame interactions for Cases 1-4 are shown in Figures 4a-d, respectively. The temporal evolution of simulated OH LIF signals was computed using species mole fractions and temperatures obtained from the DNS to facilitate comparisons with the experiment. The addition of NO promotes the formation of an autoignition kernel as in the experiments. However, the time required for the extinction/re-ignition process in the simulations is slightly longer than in the experiments. This discrepancy may result from the sensitivity of extinction/re-ignition timing to uncertainties in the chemical mechanism and the transport properties, in addition to uncertainties in the measured temperatures and velocities at the boundaries. Figures 4b-c show that the addition of H₂O to the NO-doped air delays the formation of the autoignition kernel. For Cases 3 and 4 (Figures 4c-d), local extinction and re-ignition occur in a similar manner, confirming that the thermal effect of the additional water vapor is negligible.

The numerical results reveal the competitive effects of NO and H₂O on the consumption of HO₂ and the production of OH. An elementary reaction rate analysis confirms that NO doping enhances OH generation by forming a catalytic cycle via $\text{NO} + \text{HO}_2 \rightleftharpoons \text{NO}_2 + \text{OH}$ (R28) and $\text{NO}_2 + \text{H} \rightleftharpoons \text{NO} + \text{OH}$ (R27) during the ignition induction period. Figure 5 shows the effects of NO and H₂O addition on the temporal evolution of OH mole fraction and the OH production rates of reactions R27 and R28 at the location of maximum OH mole fraction along the burner centerline. For the case with only NO addition, the degree of reduction in OH mole fraction during extinction at ~25 ms is far less, and the delay time for re-ignition is shorter than for the other two cases. The small amount of NO addition enhances OH production during the ignition induction period by consuming HO₂ and providing OH branching via R27 and R28. By contrast, the H₂O addition counteracts this catalytic effect and significantly delays re-ignition. The inhibiting effect of H₂O results from its relatively large chaperon efficiency in the three-body recombination reaction, $\text{H} + \text{O}_2 + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$, which increases the production rate of HO₂.

This combined experimental and numerical study of hydrogen counterflow flames provides insight into the complex interactions between transient flows and flame ignition. The accurate prediction of extinction and ignition dynamics requires the development of chemical mechanisms that are accurate over a wide range of thermochemical conditions. Current research efforts are focusing on extinction and re-ignition of a wide range of hydrocarbon fuels with various additives.

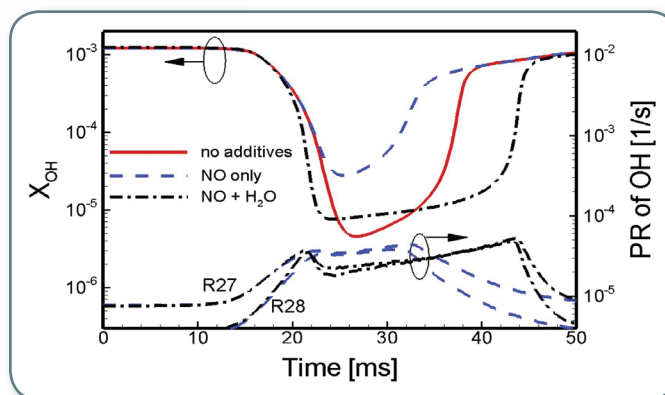


Figure 5. Computed temporal evolution of maximum OH mole fraction along the burner axis and the production rate of OH from reactions R27 and R28 at the location of maximum X_{OH}

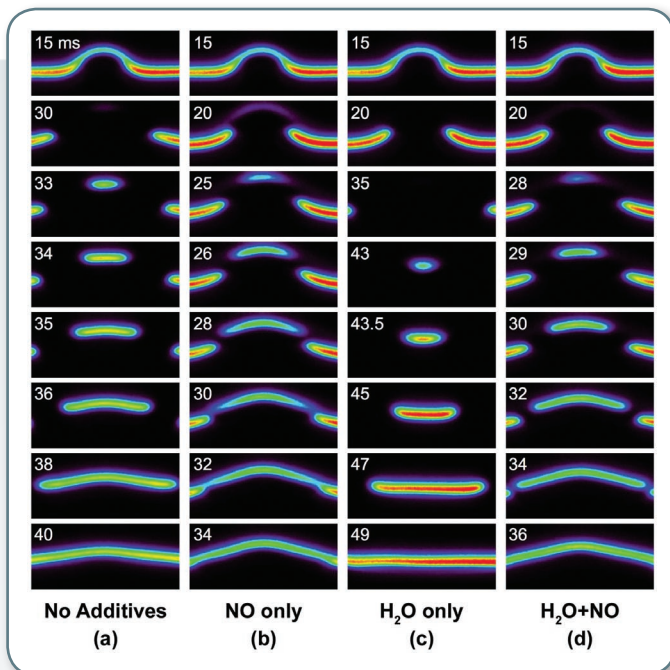


Figure 3. OH LIF measurements of the flame-vortex interaction with and without additives. Fuel stream: $X_{\text{H}_2} = 0.115$, $X_{\text{N}_2} = 0.885$, Air stream: $T_{\text{air}} = 960$ K. (a) no additives (b) doping of air with 160 ppm NO (c) doping of air with 1.2% water vapor (d) doping with water vapor and NO.

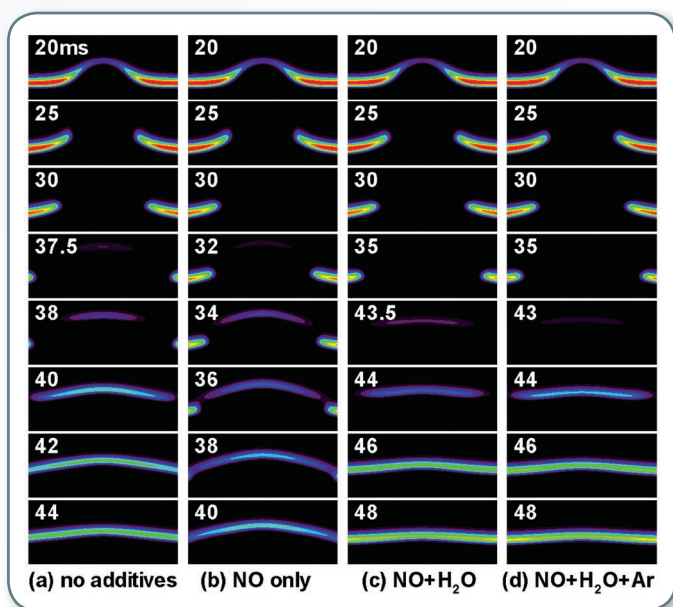


Figure 4. Simulated OH LIF signals from DNS calculations of the flame-vortex interaction with and without additives. Fuel stream: $X_{\text{H}_2} = 0.115$, $X_{\text{N}_2} = 0.885$, Air stream: $T_{\text{air}} = 960$ K. (a) No additives (b) doping of air with 160 ppm NO (c) combined doping with 2.6% water vapor and 160 ppm NO (d) doping with water vapor, NO, and 3.6% Ar.

Improving low-load combustion in HCCI engines (continued)

(Continued from page 2)

fication increases progressively with a delayed start of injection. However, the mixing rate is faster with the multi-hole injector because it produces a more uniform mixture than the hollow-cone injector for any given injection timing. As a result, injection can be delayed until 315°CA with the multi-hole injector while still maintaining NO_x emissions well below US 2010 standards, whereas the hollow-cone injector can only be delayed until 300°CA, as indicated by the images outlined in red in the figure. Examination of these images shows a maximum ϕ of 0.6 to 0.7, in agreement with the onset of the sharp rise in NO_x emissions observed under fired conditions in the metal engine. For both image sequences, later injection timings produced higher

equivalence ratios, in agreement with the large increase in NO_x emissions (Figures 1 and 2).

These results show that appropriate adjustment of the parameters controlling fuel/air mixing can significantly improve the combustion-efficiency/NO_x tradeoff for low-load HCCI, providing combustion efficiencies up to 92.5%. In general, faster mixing rates combined with later injection timings were found to give better performance. This finding suggests that development of fuel-injection systems with even faster mixing could further improve combustion efficiency and provide more robust operation at low-loads.



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