W4P076: PAH OXIDATION WITH O$_2$ IN SOOT PARTICLES
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This work aims to incorporate a detailed PAH oxidation reaction mechanism proposed by A. Raj et al. (2012) into a detailed kinetic Monte Carlo model describing the evolution of PAH molecules, modified from the model by A. Raj et al. (2009). The mechanism is reduced into a number of one-step jump reactions through investigation in a batch reactor environment and route path analysis, and then fitted to counter-flow diffusion flame data A. Raj et al. (2011). Finally, with the inclusion of the one-step jump oxidation reactions in the PAH evolution model, coupled with a highly detailed soot model will be used in the investigation of PAH oxidation in soot particles in flames.

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W4P077: LINEAR-EDDY MODEL FORMULATED PROBABILITY DENSITY FUNCTION FOR PREMIXED COMBUSTION
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A modified version of Linear-Eddy Model (LEM) is used to generate Probability Density Functions (PDF) for a product-based reaction progress variable in an inflow-outflow, premixed, turbulent reacting field. The LEM PDFs at several axial locations of the flame are compared to PDFs extracted from Direct Numerical Simulations (DNS). LEM demonstrates the ability to better capture turbulent effects than previously suggested PDF models for the prescribed configuration. LEM is then used to simulate a premixed, turbulent methane/air v-flame produced by the Cambridge slot burner. The model is able to produce all the salient features observed from the temperature-based experimental PDFs. The stochastic nature of LEM enables it to reproduce the overall behaviors of turbulent reactions inexpensively and qualitatively. This makes LEM ideal for data preprocessing for Conditional Source-Term Estimation.

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W4P078: DETAILED NUMERICAL SIMULATION OF SYNGAS COMBUSTION UNDER PARTIALLY PREMIXED COMBUSTION ENGINE CONDITIONS
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Two-dimensional direct numerical simulation (2-D-DNS) is performed to study syngas/air combustion under partially premixed combustion (PPC) engine conditions. Detailed chemical kinetics and transport properties are employed in the study. The effect of piston compression and multiple stage fuel injections is taken into account in the simulations. The fuel, a mixture of CO and H$_2$ with a 1:1 molar ratio, is introduced to the domain at two different times, corresponding to the multiple injection strategy of fuel used in PPC engines. It is found that the ratio of the fuel mass between the second injection and the first injection affects the combustion and emission process greatly; there is a tradeoff between emissions of NO and emissions of CO when varying the fuel mass ratio. The ignition zone structures under different fuel mass ratios share similarity. A premixed burn region and a diffusion burn region are identified. The premixed burn region ignites first, followed by the ignition of mixtures at the diffusion burn region, and finally a thin diffusion flame is formed to burn out the remaining fuel. NO is mainly produced in the premixed burn region, and partly from the diffusion burn region in mixtures close to stoichiometry, whereas unburned CO emission is mainly from the diffusion burn region. An optimization of the fuel mass in the two regions can offer a best tradeoff between NO emission and CO emission. The effect of initial temperature and turbulence on the premixed burn and diffusion burn regions is investigated.

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W4P079: DUAL PUMP CARS MEASUREMENTS IN A SUPERSONIC COMBUSTING FREE JET
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Successful design of hypersonic air-breathing engines requires new computational fluid dynamics (CFD) models for turbulence and turbulence-chemistry interaction in supersonic combustion. Unfortunately, not enough data are available to the modelers to develop and validate their codes, due to difficulties in taking measurements in such a harsh environment. Dual-pump coherent anti-Stokes Raman spectroscopy (CARS) is a non-intrusive, non-linear, laser-based technique that provides temporally and spatially resolved measurements of temperature and absolute mole fractions of N$_2$, O$_2$ and H$_2$ in H$_2$-air flames. A dual-pump CARS instrument has been developed to obtain
measurements in supersonic combustion and generate databases for the CFD community. Accuracy, precision and spatial resolution of the instrument has been determined experimentally. A small, axis-symmetric supersonic combusting coaxial jet facility has been developed to provide a simple, yet suitable flow to CFD modelers. The facility provides a central jet of hot “vitiated air” simulating the hot air entering the engine of a hypersonic vehicle flying at Mach numbers between 5 and 7. Three different silicon carbide nozzles, with exit Mach number 1, 1.6 and 2, are used to provide flows with the effects of varying compressibility. H₂ co-flow is available in order to generate a supersonic combusting free jet. Dual-pump CARS measurements have been obtained for varying values of flight and exit Mach numbers at several locations. Approximately one million dual-pump CARS single shots have been collected in the supersonic jet for varying values of flight and exit Mach numbers at several locations. Data have been acquired with a H₂ co-flow (combustion case) or a N₂ co-flow (mixing case). The experimental results for the mixing test cases show that increased compressibility reduces the shear layer spreading rate, and the turbulence fluctuations, in agreement with what was observed in previous experimental work. The dual-pump CARS measurements in the reacting test cases show that the heat released from the combustion strongly limits the growth of the co-flow shear layer, and the mixing of the center jet. Examination of the standard deviation and of the co-variances profiles is very useful in determining where significant mixing and combustion are occurring. The experimental results are in agreement with what was previously observed or predicted, but the relevance of the acquired data-set lays in providing accurate quantitative measurements of the distributions of mean and fluctuation parameters.

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W4P080: CHANGES OF GAS VELOCITIES IN PASSING THROUGH FLAMELETS
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An attempt has been made to examine the effects of flamelets on the local flow in turbulent premixed flames in a reaction-sheet regime. Vectors of the flamelet motion and of gas velocity have been measured simultaneously by use of a four-element electrostatic probe and a three-component LDV system. Measurements were made at the position of maximum ion current on the centerline of the turbulent flame brush. For planar flamelets, use of the four-element electrostatic probe simultaneously with a three-component LDV theoretically can provide complete fluid-mechanical information for motion of the flamelet and the gas velocities separately and simultaneously.

It was found to be possible, during each flamelet passage, to rotate the coordinate system about a vertical axis so that the flamelet and all gas velocity vectors remained very nearly in the same vertical plane, thereby implying locally nearly two-dimensional motion, insofar as the influence of the gas expansion on the gas velocity is concerned. In the local plane of motion, the observed changes in gas velocity caused by flamelet passage exhibited a downward component for upward moving flamelets with the fresh mixture above the burnt gas and an upward component for upward moving flamelets with the burnt gas above the fresh mixture, consistent with the expected gas expansion through the flamelet. Moreover, within the accuracy of the LDV measurements, profiles of changes of the component of gas velocity normal to the flamelet agreed with velocity profiles calculated for steady, planar, unstretched, premixed laminar flames. These results indicate relatively little distortion of laminar flamelet structures in the turbulent flame brush at these turbulent intensities of about 5 %, although CO oxidation may be slowed.

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