"Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry"
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Direct Numerical Simulation of Non-Premixed Flame-Wall Interactions

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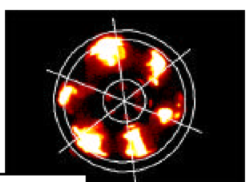
• Motivation

- **Engine applications:** Flame-wall interactions (FWI) are observed in many combustion systems (*i.e.* IC engines, micro-scale combustors); FWI result in decreased performance, both in terms of thermal efficiency and pollution propensity;
- **Fire applications:** FWI are also observed in many fire configurations, whenever the flame develops near a solid (inert/flammable) surface (*i.e.* wall fires, impinging flames); FWI contribute to the wall surface heat transfer (*i.e.* to the fuel pyrolysis) and to the thermal loading experienced by solid structures;
- **CFD modeling:** FWI are simply neglected in current engineering-level CFD models (wall boundary layer models, developed for inert flows, are inadequate).



Diesel engine

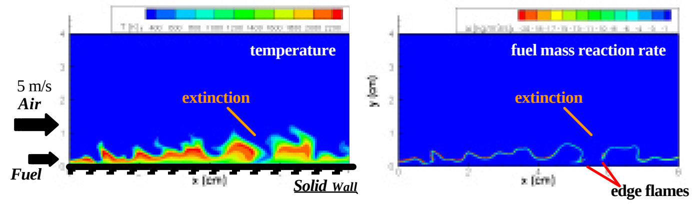
Wall fire

• Approach:

- Use Direct Numerical Simulation (DNS) to bring basic information on the interaction of non-premixed flames with cold solid wall surfaces;
- Leverage SciDAC collaboration on DNS solver called S3D: Univ. Michigan (H. G. Im), Univ. Wisconsin (C. Rutland), Sandia National Laboratories (J. H. Chen).

• Main features of DNS solver (S3D):

- Navier-Stokes solver; fully compressible flow formulation; pseudo-compressibility method to handle acoustic stiffness;
- High-order finite difference (8th order); high-order explicit Runge-Kutta time integrator (4th order);
- Characteristic-based boundary condition treatment (NSCBC);
- Parallel (MPI-based, excellent scallability);
- Flame modeling: detailed fuel-air chemistry (CHEMKIN-compatible); simplified soot formation model; thermal radiation model (Discrete Ordinate/Discrete Transfer Methods); Lagrangian particle model to describe dilute liquid sprays.



DNS configuration: a non-premixed C_2H_4-air flame embedded in a turbulent boundary layer that develops near a cold wall surface

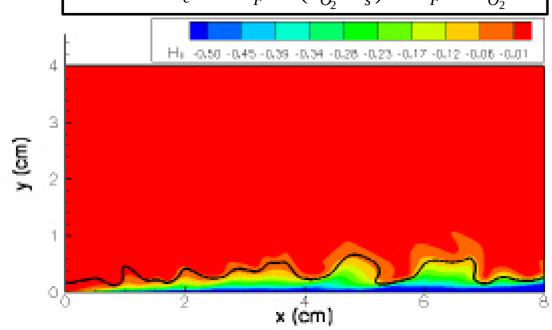
• Observations of near-wall flame dynamics:

- Multiple flame sheets; flame quenching events; development of a thin cold sub-region near the wall;
- Quantification of the wall surface heat flux (convective heat transfer): up to 90 kW/m^2.

• Analysis:

- **Description of flame structure:** introduction of a new variable H called excess enthalpy to measure deviations from adiabatic flame behavior:

$$H = \frac{c_p(T-T^\infty)}{\Delta H_c}\left(\frac{1}{Y_F^\infty} + \frac{1}{(Y_{O_2}^\infty / r_s)}\right) + \frac{Y_F}{Y_F^\infty} + \frac{Y_{O_2}}{Y_{O_2}^\infty} - 1$$



Instantaneous snapshot showing the wall-cooled region (*H*-contours in color) and the flame location (black line)

- **Modified flame extinction criterion:**

$$c_{st} \geq \underbrace{c_{st,ext}^{ad}}_{\text{extinction value (adiabatic case)}} \times \exp(\underbrace{b}_{\text{Zeldovich number}} \times \underbrace{H_{st}}_{\text{excess enthalpy at flame location}})$$

• Conclusion: New combustion science!

- **Exploration:** DNS allows fundamental observations of FWI, *i.e.* the dynamics of the wall-cooled region, flame extinction events, peak wall heat flux events;
- **Analysis and Modeling:** DNS also promotes new theoretical developments, *i.e.* in the present study, an extension of the classical description of flame structure to the case of non-adiabatic combustion.