LES Modeling for IC Engines

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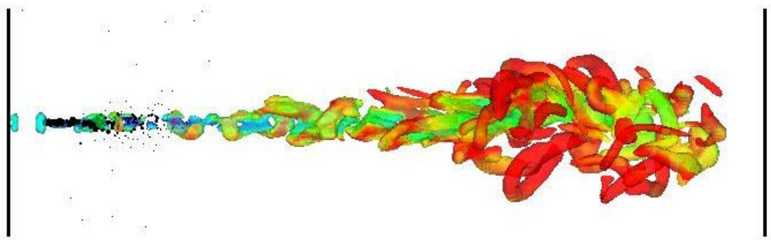
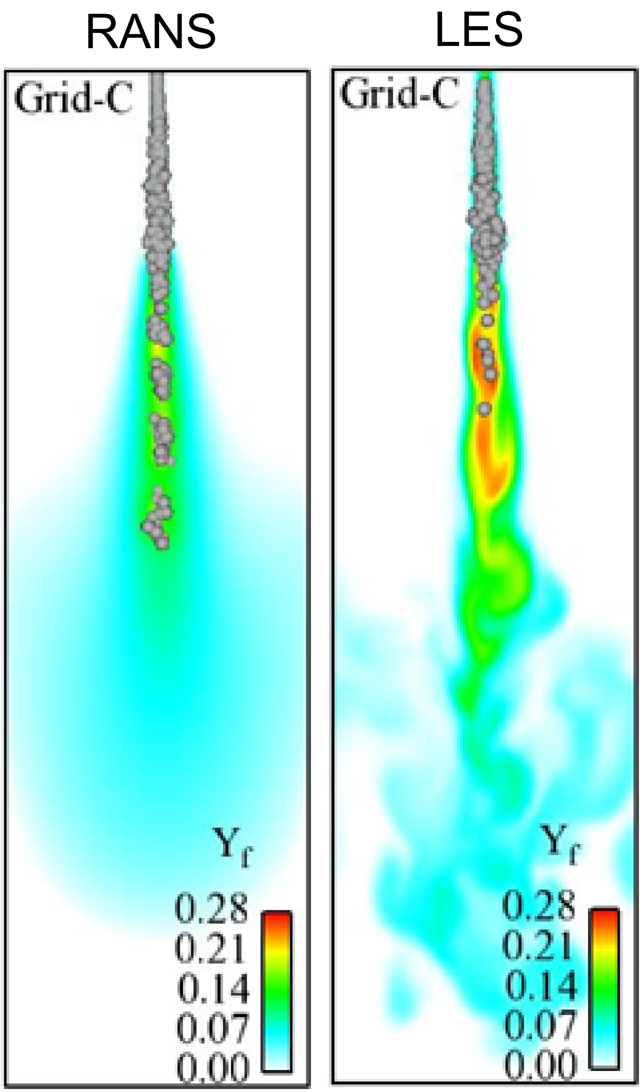


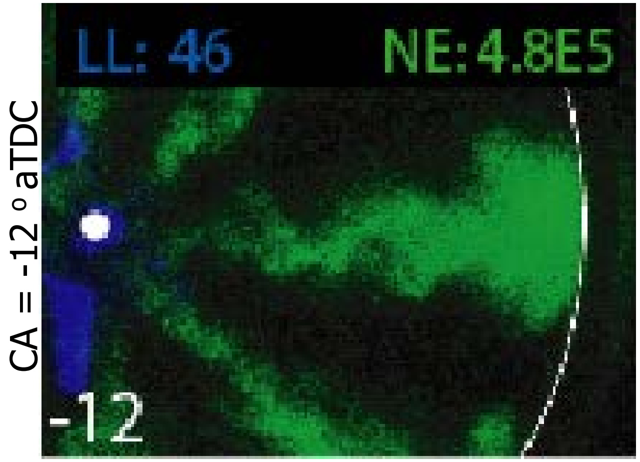
LES Introduction

- Large Eddy Simulation
  - Next generation of turbulence modeling
- Concept:
  - RANS uses ensemble averaging
  - LES uses local spatial averaging (filtering)
  - Achieved by different sub-models
- Intent
  - Retain more flow structure on grid
  - Better predictive capability
  - Capture more details by simulating more flow structures

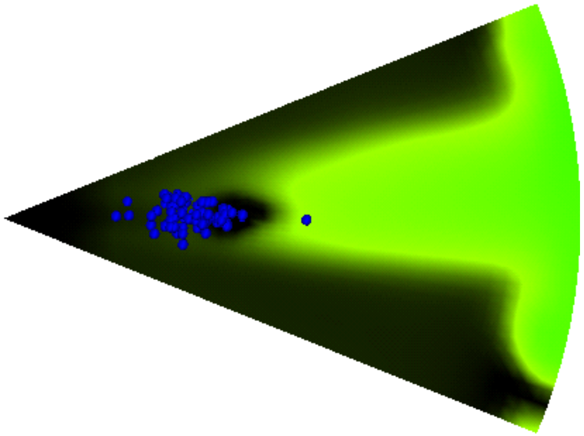


Better Predictive Capability

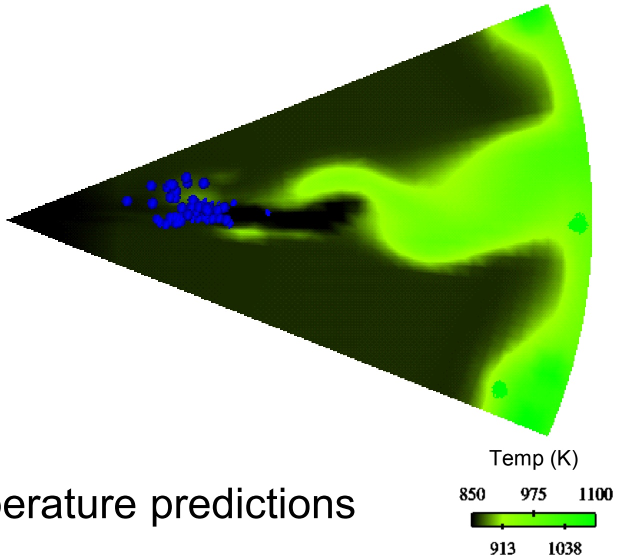
Experiment



RANS



LES



- Ignition chemiluminescence compared with temperature predictions

LES Advantages

<u>Increased design sensitivity</u>

Capture more flow instabilities

Better response to geometric details

Address wider range and more subtle design conditions

<u>Study new phenomenon</u>

Cycle-to-cycle variability

(Experimental images courtesy Singh et al., 2006)

Practicalities of LES in Engines

- LES is:
  - NOT: Just an LES turbulence model
  - NOT: Turn-key for IC engine applications
- Need reasonable computational times
  - Limits grid density
  - Requires accurate sub-models
- Complex physics
  - Sub-grid models for
    - Turbulence
    - Combustion
    - Scalars
    - Sprays
    - Walls, injectors, etc.

LES versions required

LES Sub-Models for Engines

- <u>Tier 1 models: Available for use</u>
  - Turbulence *
  - Combustion
  - Scalars
  - Sprays: far field effects

- 0 – equation
- 1 – equation
  - Viscosity
  - Non-viscosity

- <u>Tier 2 models: Need work</u>
  - Emissions
  - Wall effects and wall heat transfer
  - Sprays, sprays, sprays
    - Nozzle effects, breakup, atomization

LES Modeling Technologies

- Scale similarity
  - Use big ‘whorls’ to help model small ‘whorls’
- Dynamic procedure
  - Obtain sub-model coefficients from solution
- Approximate de-convolution
  - Reverse filter: estimate small scales

Examples

- Combustion modeling
- Spray modeling
- Wall heat transfer modeling

Mixing-Controlled Detailed Chemistry (MCDC) Model

- Modifies chemistry solution with mixing time scale
- Based on 'Kong-Reitz' model formulation [*Kong et al*, 2002]:

$$\dot{\varpi}_i = \frac{1}{1+Da}\dot{\varpi}_{DCS,i}$$

- Damkohler number: $Da = \frac{\tau_{mixing}}{\tau_{DCS}}$

- Mixing time scale: $\tau_{mixing} \approx 1/\chi_{sgs}$

DCS = Direct Chemistry Solver (Chemkin or equivalent)

DCS reaction rate for species i:

$$\dot{\varpi}_{DCS,i}$$

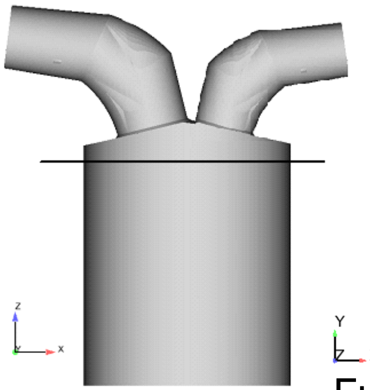
$$\chi_{sgs} = S(\mathrm{Re}_{sgs})\left(\widehat{\frac{\partial\tilde{Z}}{\partial x_i}\frac{\partial\tilde{Z}}{\partial x_i}} - \frac{\partial\hat{\tilde{Z}}}{\partial x_i}\frac{\partial\hat{\tilde{Z}}}{\partial x_i}\right)$$

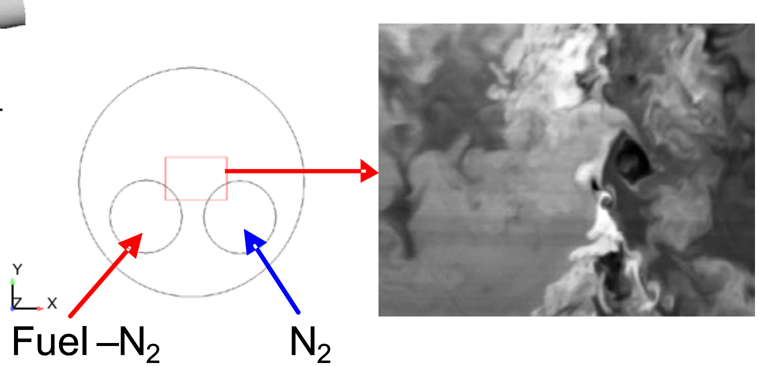
Dynamic scale similarity model: χ_{sgs}

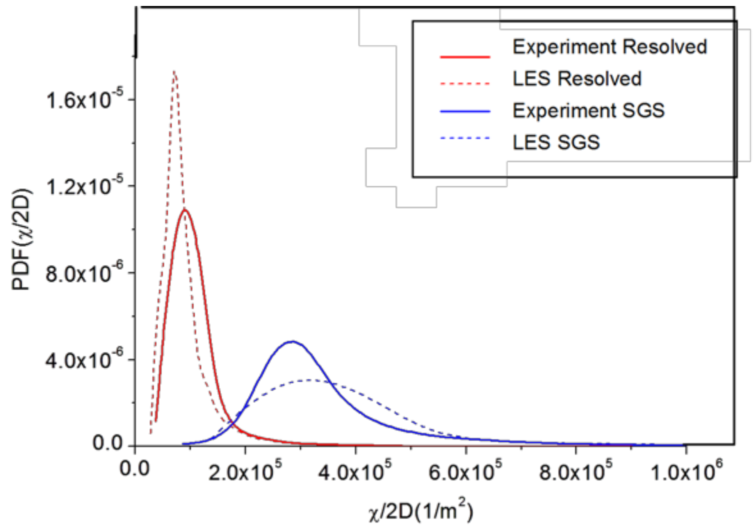
Subgrid χ Model Validation

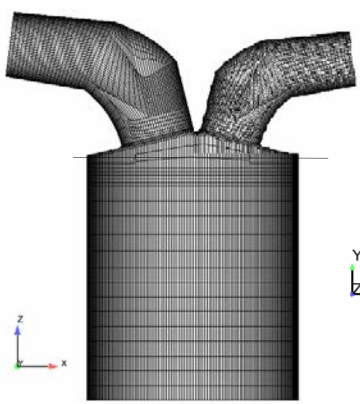
- Engine comparisons
  - PLIF experiments of Peterson and Ghandhi

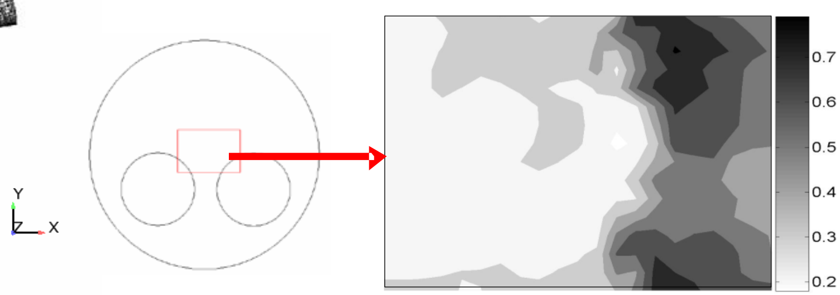
Ensemble PDF of resolved and subgrid scalar dissipation











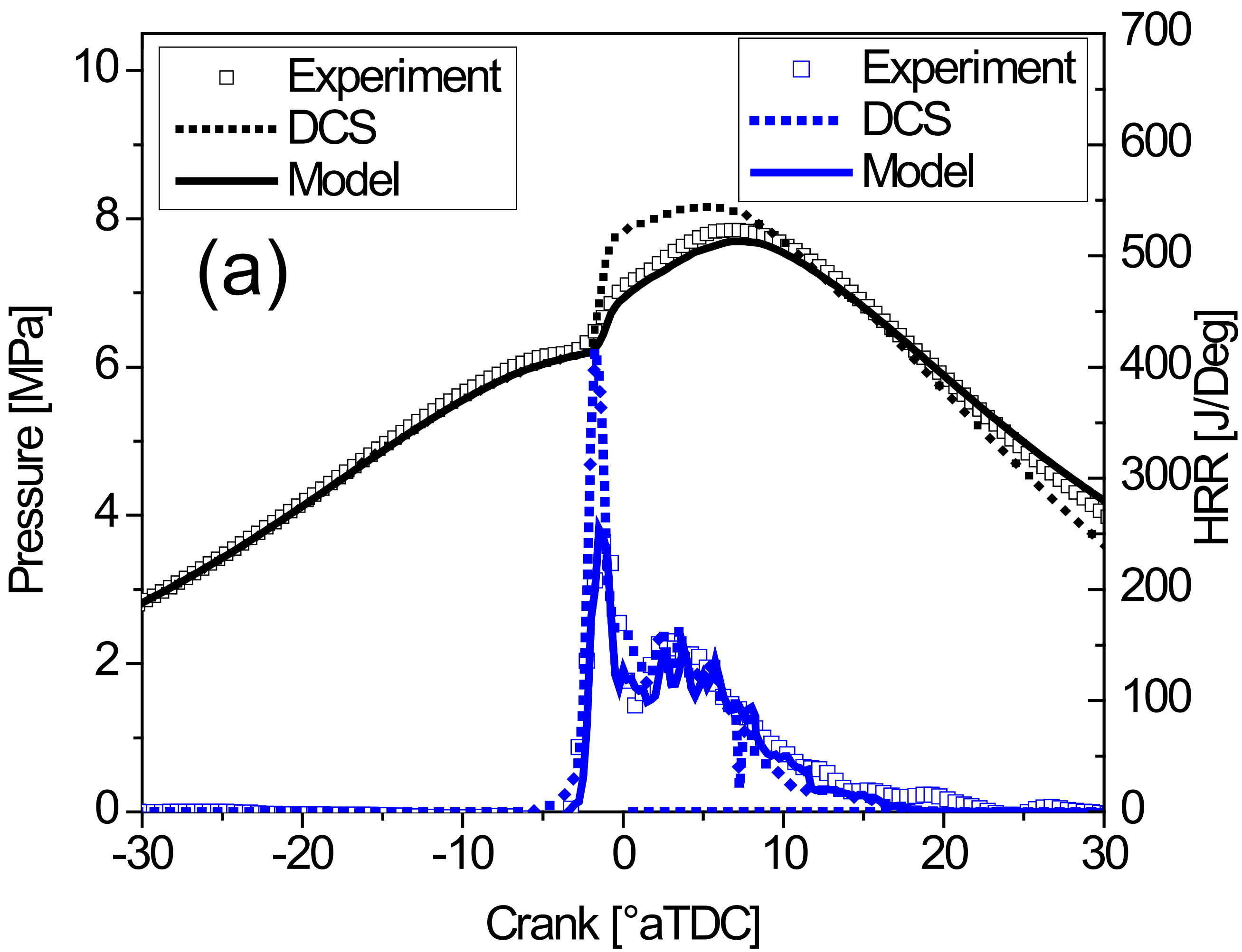
125-cycle experimental
10-cycle LES simulations

Tin = 323 K, 240 bTDC. Sample domain: 19.5 x 15.2 mm.

MCDC Combustion Model Validation

Sandia Cummins N-14 optical engine

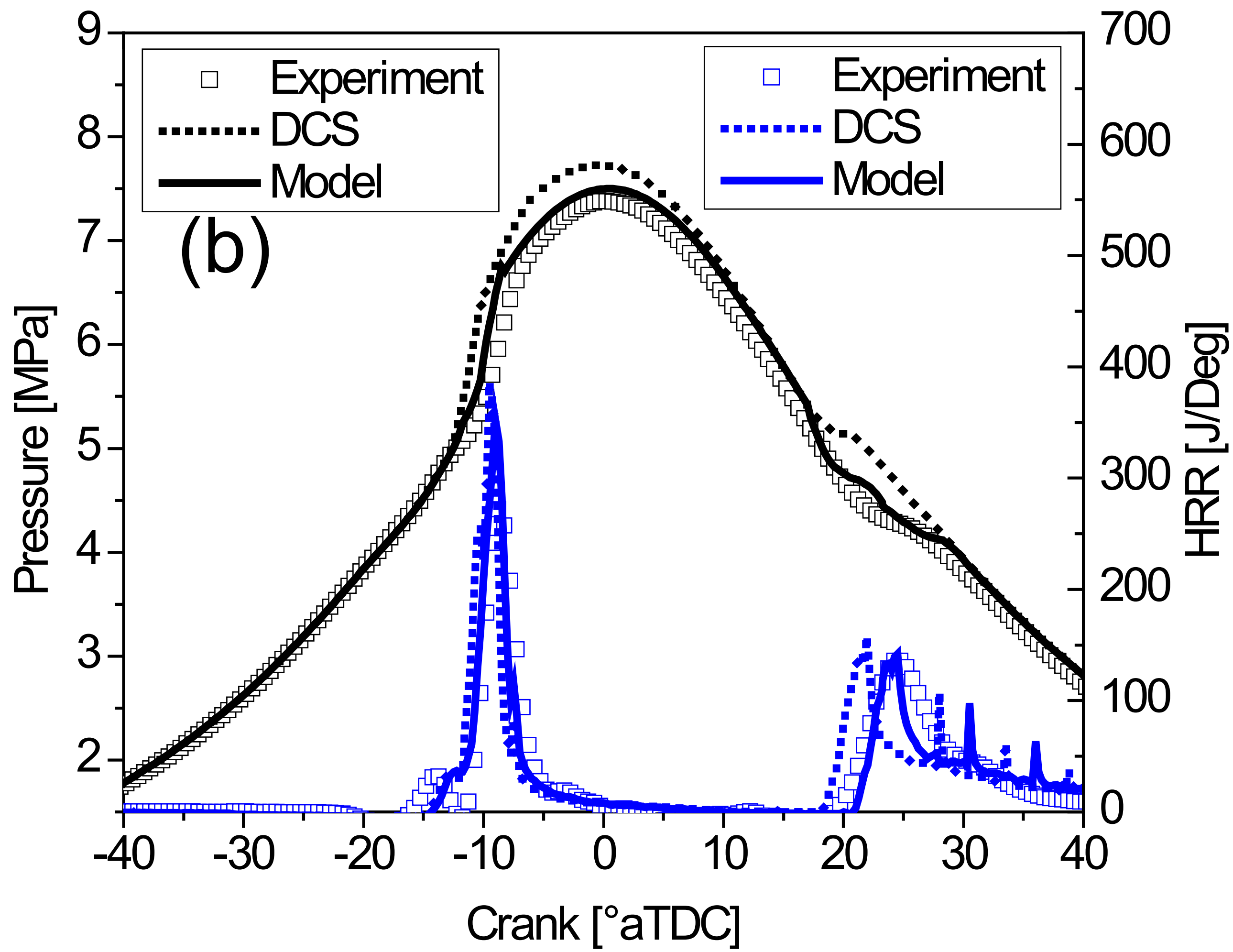
Engine speed [RPM]	**1200**
IMEP [bar]	**4.4**
Injection pressure [bar]	**1200**
Intake temperature [°C]	**111**
SOI [° ATDC]	**-7**



MCDC Combustion Model Validation

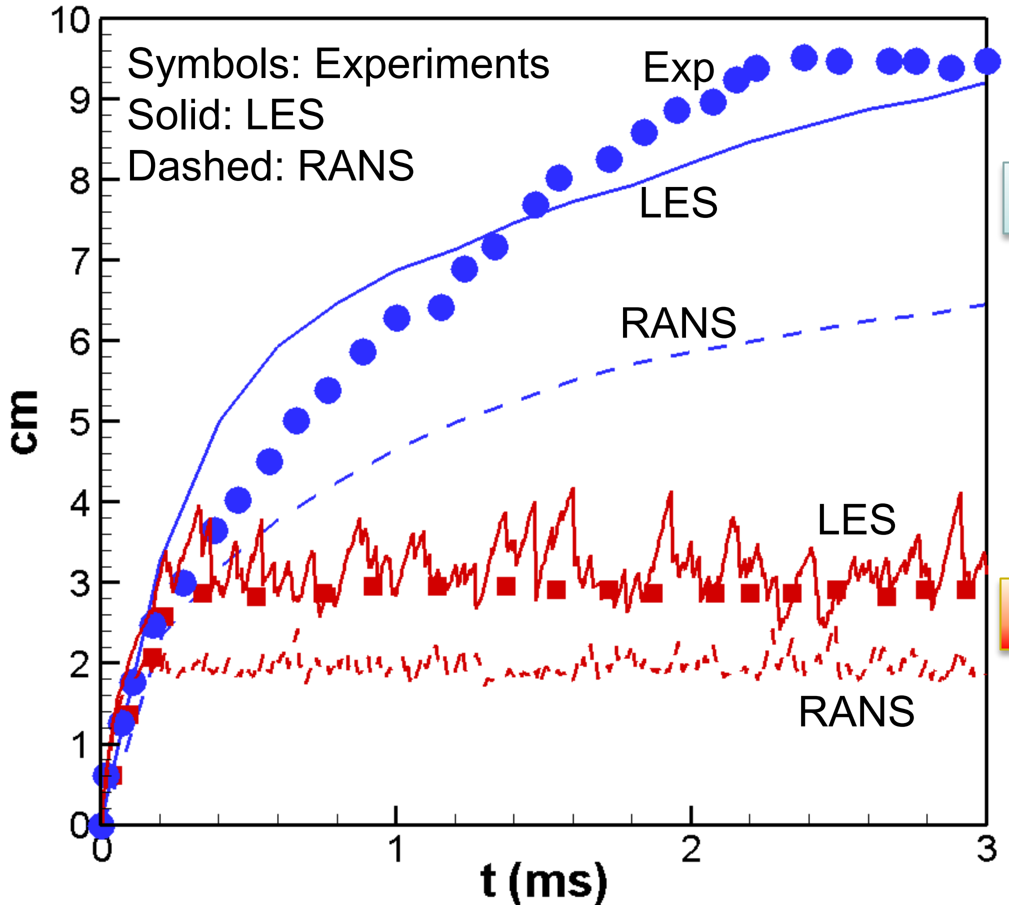
Sandia Cummins N-14 optical engine

Engine speed [RPM]	**1200**
IMEP [bar]	**4.6**
Injection pressure [bar]	**1600**
Intake temperature [°C]	**90**
SOI [° ATDC]	**-22,+15**



Spray Modeling

- Key component for LES spray modeling: <u>spray source term</u> in sub-grid kinetic energy equation: used approximate de-convolution
- Liquid and vapor penetration: LES and RANS show similar global results



Vapor penetration

Liquid penetration

- Injection pressure: 135 MPa
- Nozzle diameter: 246 μ
- Ambient density : 30.2 kg/m3
- Ambient temperature: 1000 K

High Flame Lift-off Case

0.0000s ASOI

- Coherent structures: yellow
- Cool flame: blue (CH_20)
- High temperature reactions: red (OH)

✓ Cool flame (CH_2O) evolves with the CS
✓ Long cool flame period

Fuel Injection	1163 bar
Fuel, temperature	$C_{14}H_{30}$, 408 K
Ambient pressure	22.7 bar, 1100 K
Ambient density [kg/m^3]	7.17

Low Flame Lift-off Case

0.0000s ASOI

- Coherent structures: yellow
- Cool flame: blue (CH_20)
- High temperature reactions: red (OH)

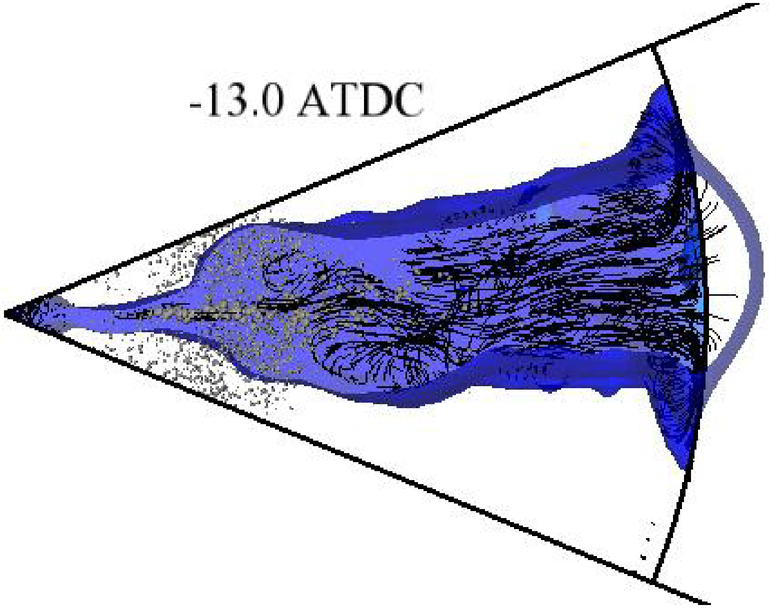
✓ Cool flame is inside high temperature reaction zone

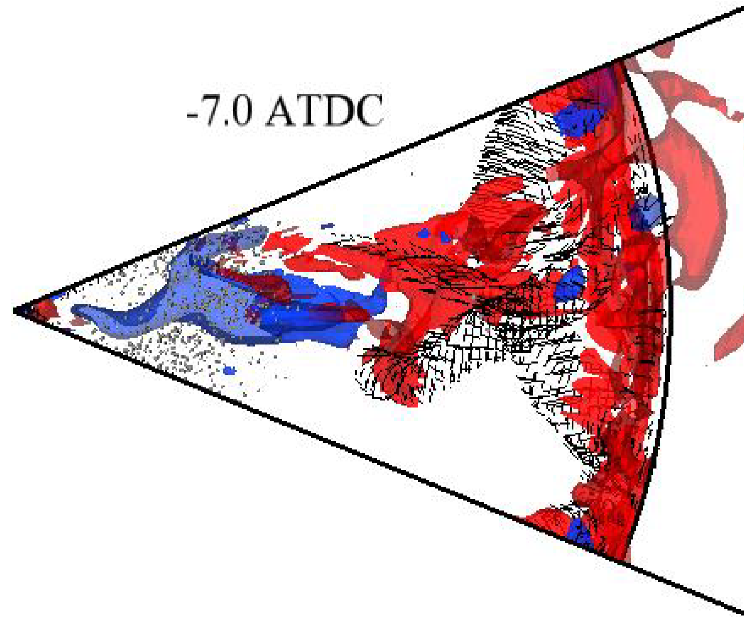
✓ Cool flame has a steady penetration (~1 ms ASOI)

✓ High temperature reaction zone evolves with the CS

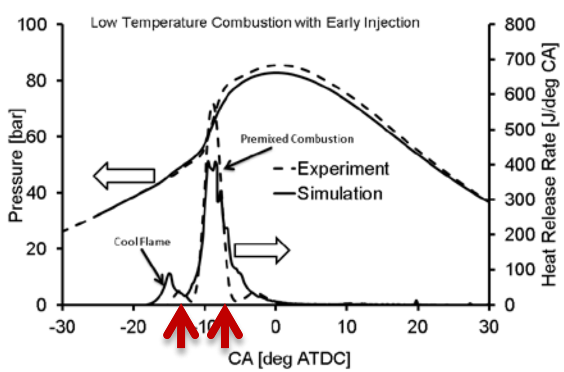
Fuel Injection	1163 bar
Fuel, temperature	$C_{14}H_{30}$, 408 K
Ambient pressure	64 bar, 1200 K
Ambient density [kg/m^3]	18.58

Engine Case: LTC Early Injection

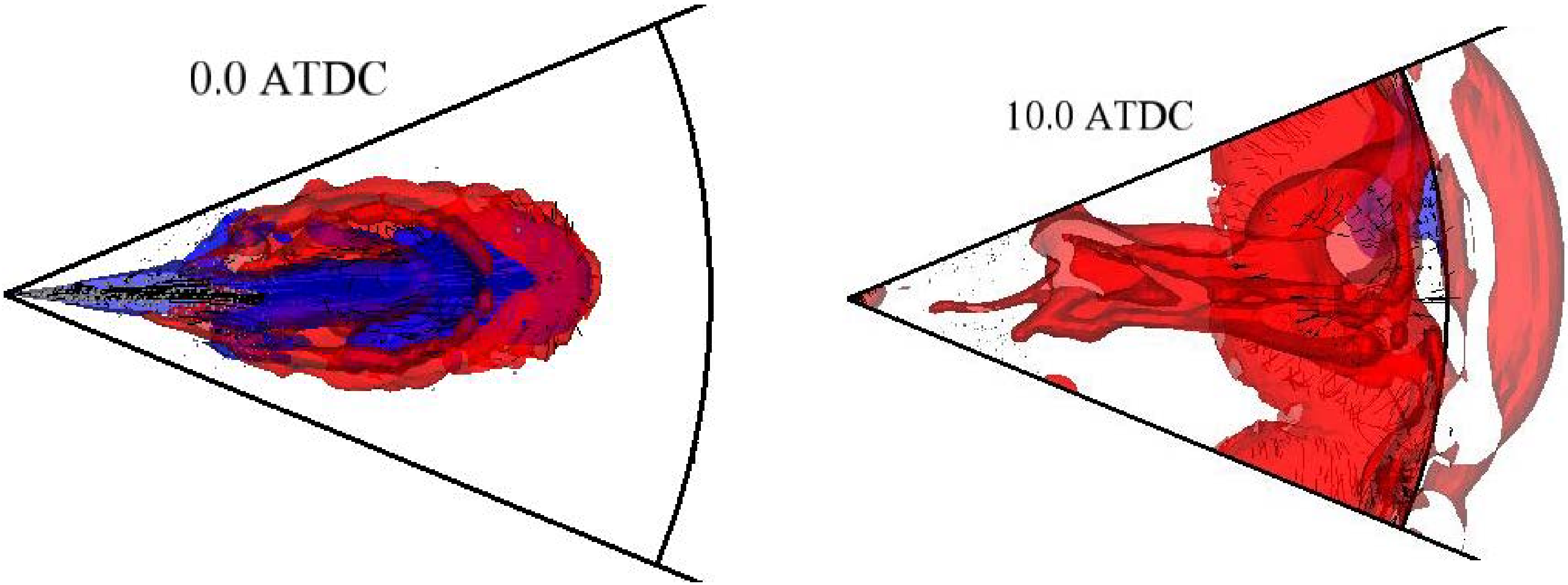




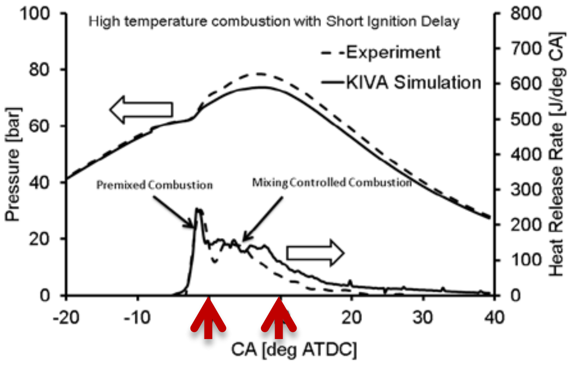
Blue: Cool flame (CH20)
Red: High temperature reaction zones (OH)
Grey: Droplets
Black: Velocity vectors on CS



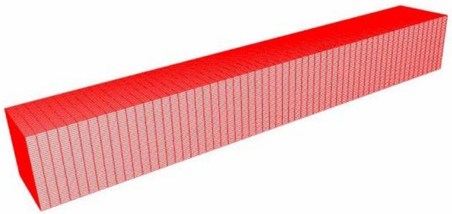
Engine Case: Short Ignition Delay



Blue: Cool flame (CH20)
Red: High temperature reaction zones (OH)
Grey: Droplets
Black: Velocity vectors on CS

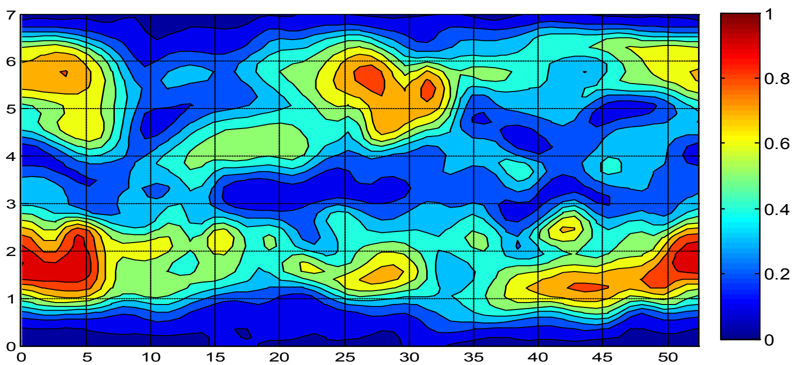


Wall Modeling: Channel Flow

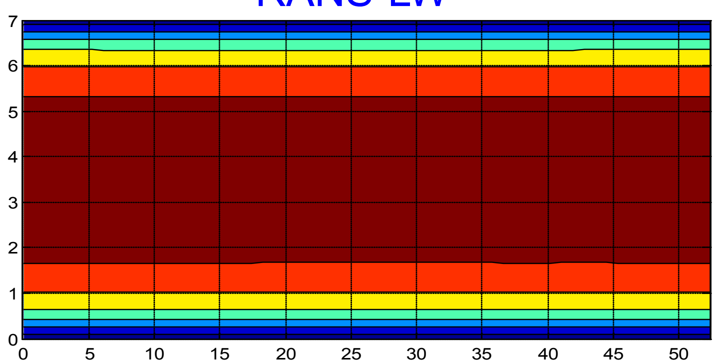


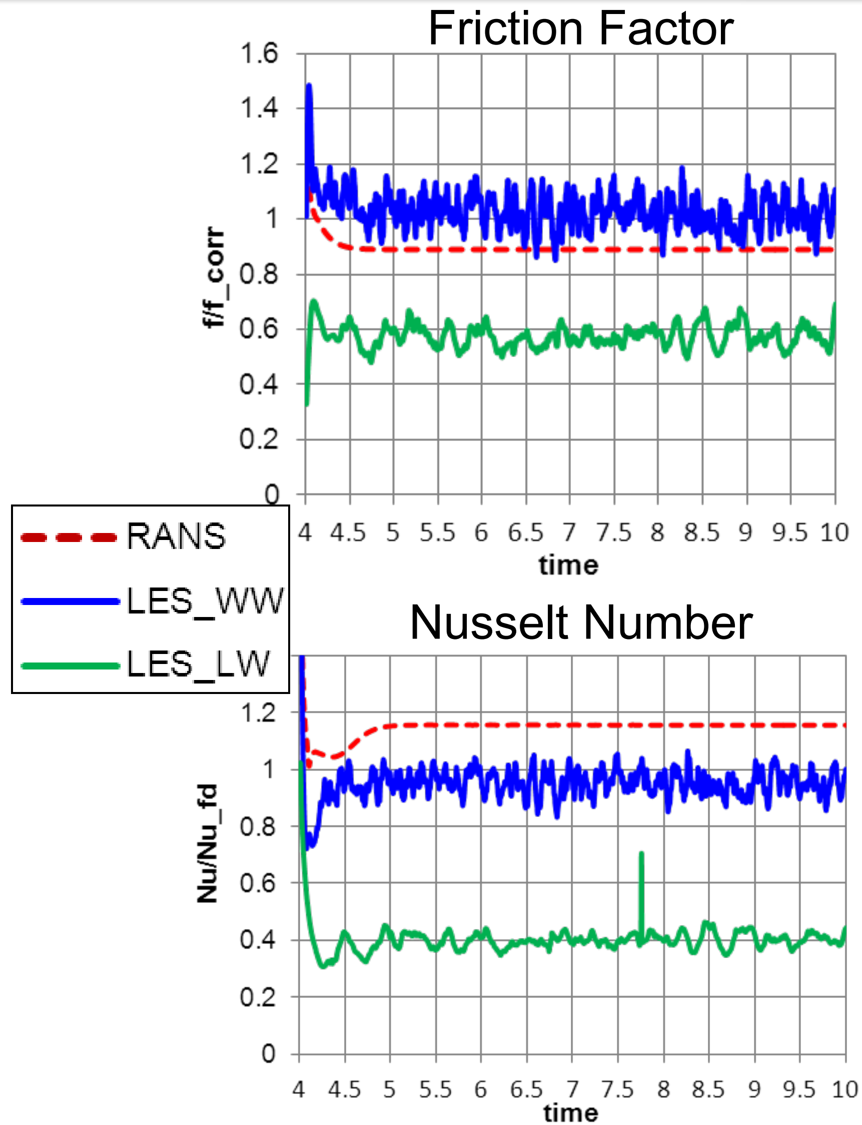
Wall Heat Flux

LES-WW

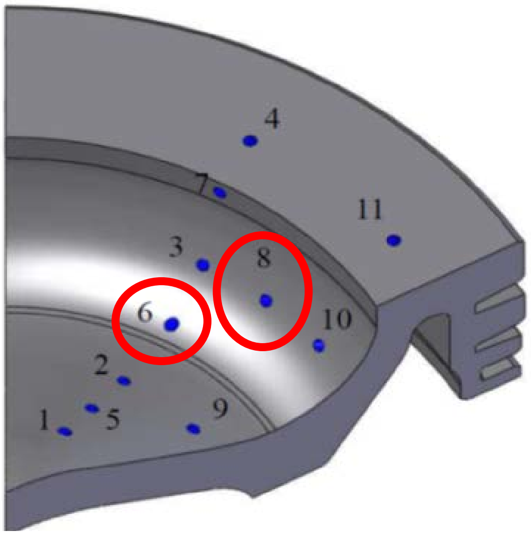


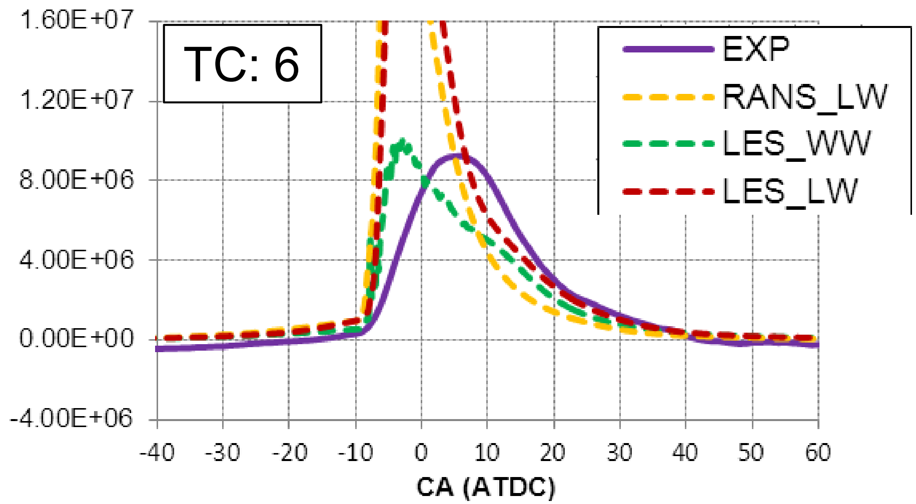
RANS-LW

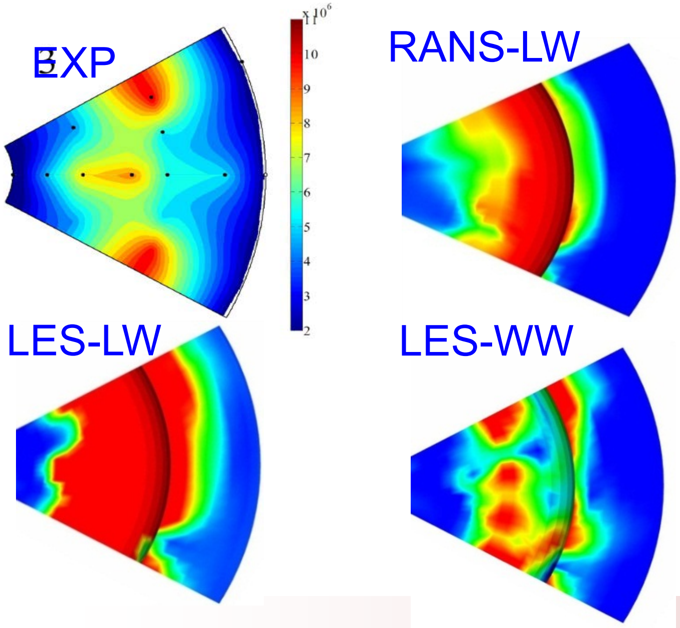


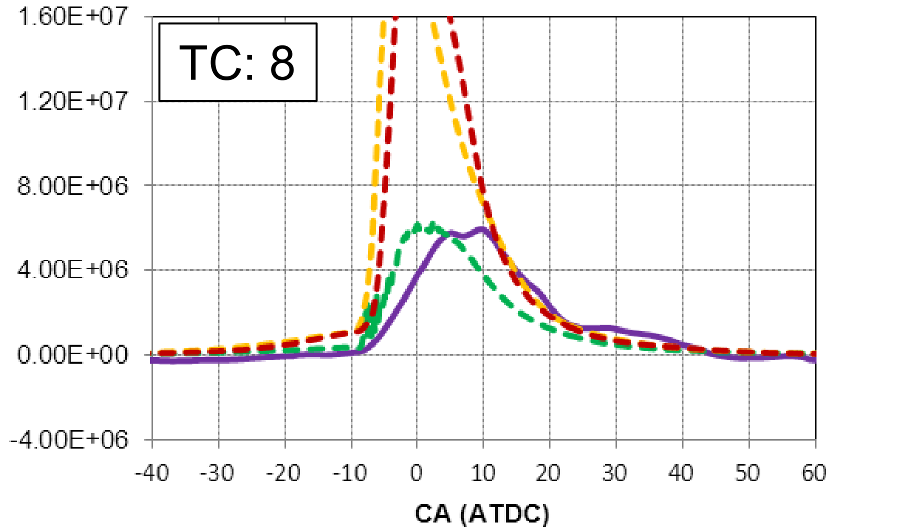


Engine Wall Heat Transfer









Summary

- LES can increase accuracy and sensitivity
- LES for engine modeling is here now
  - Requires accurate sub-models
  - Requires very knowledgeable users
- Current efforts on improvements
  - Sprays: nozzle interior, near nozzle
  - Appropriate use: multiple cycles, new analysis techniques, validation
- Additional information:

"Large Eddy Simulations for Internal Combustion Engines – A Review," Rutland, *International Journal of Engine Research*, 2011, Vol. 12 (5), pp 421-451 DOI: 10.1177/1468087411407248.

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Thank You