LES of Diesel Sprays Using Advanced Computational Methods and Models for Mixture and Emission Formation

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LES for Internal Combustion Engine Flows [LES4ICE]
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General Issues in Diesel Engine Combustion

- Geometry
- Spray
  - Nozzle flow
  - Primary and secondary breakup
  - Wall impingement
  - Evaporation
- Surrogate fuel chemistry needs to describe
  - Auto-ignition
  - NOx formation
  - Soot precursor (PAH) formation
  - Heat release
- Combustion model needs to handle
  - Detailed chemistry of multi-component fuels
  - Split injection
  - Heat transfer
and describe
  - Pollutant formation
  - Auto-ignition
  - Premixed/diffusive burning

- Complex piston shape
- Piston shape important for emissions
- Moving walls
  - Piston
  - Valves
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- Modeling spray inside the nozzle
  - Cavitation
- Injection rate very important for emissions
- No model for primary breakup
- Wall film models
  - Film development
  - Wall film evaporation
- Evaporation depends on local droplet concentration
- Evaporation/combustion interaction
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- **Surrogate fuels for Diesel**
  - n-heptane
  - n-decane
  + $\alpha$-methylnaphthalene
  - n-dodecane
  + $\alpha$-methylnaphthalene
  + branched alkane
  + cycloalkane + alkene
  + oxygenates

- **Auto-ignition chemistry typically involves hundreds of species**
- **Soot precursor chemistry complicated and not well understood**
  - Oxidation reaction
- **Reduced mechanisms essential**
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- Finite rate detailed chemistry important for emissions
- Many models cannot handle more than ~20 species
  - Transported PDF model
- Heat losses to walls lead to cold boundary layer where soot does not oxidize
- Large part of soot and UHC emissions from wall region
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- Soot model describes heterogeneous reactions of gas with soot particle phase
- Auto-ignition depends strongly on rate of mixing of fuel and oxidizer
  - Scalar dissipation rate
  - Fluctuations of mixing rate cause leading order effect in ignition delay time
- Fast premixed burn leads to
  - Pressure peaks
  - High temperature and formation of NO\textsubscript{x}
- Slow diffusive burn
  - Soot formation
  - Soot oxidation
Soot Formation in Diesel Engine Combustion

Studies in High-Pressure Combustion Chamber

• 900 K and 60 bar
• Spray and combustion characteristics (BLI, OH*)
• Soot volume fraction (LII + laser extinction)
Exemplary Images of the Spray Combustion Investigation

ASOI 400\mu s  ASOI 825\mu s  ASOI 1200\mu s  ASOI 1600\mu s  ASOI 2000\mu s

Back light illumination

ASOI 1050\mu s  ASOI 1225\mu s  ASOI 1600\mu s  ASOI 2000\mu s  ASOI 3000\mu s

OH Chemiluminescence

ASOI = After start of injection
Soot Intermittency in Turbulent Combustion

- Soot formation in spray combustion chamber
  - Five statistically equivalent instantaneous measurements
Strategy for Diesel Engine Combustion Simulation

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  - Immersed boundary with overset mesh
  - Detailed simulation of primary atomization
  - Detailed representation of chemistry
  - LES
  - Representative interactive flamelet model
  - Detailed soot model
Concept

Interfacial flow simulation

Lagrangian approach

RIF w/ 245 species
Contents

• Fundamentals and modeling of diesel spray combustion
  – Detailed simulation of primary atomization
  – Detailed representation of combustion chemistry
  – Representative interactive flamelet model
  – (Soot model)

• Simulation framework

• Results for ECN spray A constant volume chamber

• Outlook
Consistent VOF/Level Set Method

- Sharp Interface methods in complex topologies
  - Level Set (LS)
  - Volume-of-Fluid (VoF)
- Most of computational load at the interface
  - Load balancing essential
  - Unstructured/Block-Structured/AMR

Development of new numerical method:

CONSERVATION
- Mass
- Momentum

ACCURACY
- Curvature
- Flotsam/Jetsam

STABILITY
- TVD

FLEXIBILITY
- 2nd un-split VoF transport
- 2nd un-split momentum transport

Mass Conservation for Diesel Jet

- Stable for air-water density ratio
- Almost mass conserving
Mixture Formation

Detailed Simulation of Nozzle Influence on Atomization

• Experiments from Balewski et al.¹,²
• Two large-scale injectors experimentally studied using
  – Laser Doppler system
  – Phase Doppler system
  – X-ray measurements
  – High-speed photography
• Reynolds ranging from 1000 to 15500
• Weber number from 13000 to 54000

\[
Re = \frac{\rho_{\text{liq}} U_{\text{bulk}} D_{\text{nozzle}}}{\mu_{\text{liq}}}
\]

\[
We = \frac{\rho_{\text{liq}} U_{\text{bulk}}^2 D_{\text{nozzle}}}{\sigma}
\]

Prinzipdüse: Nozzle flow results

Total pipe length: 10 diameters

Comparison for V4 design, at Re = 2000

Detailed Simulation of Nozzle Influence on Atomization

Le Chenadec, V., Pitsch, H., “A conservative framework for primary atomization computation and application to the study of nozzle and density ratio effects”, Atomization and Spray, 23, 2013
Mixture Formation: Coherent Liquid

Detailed Simulation of Nozzle Influence on Atomization

Fully developed turbulent inflow

Actual nozzle inflow

Le Chenadec, V., Pitsch, H., “A conservative framework for primary atomization computation and application to the study of nozzle and density ratio effects”, Atomization and Spray, 23, 2013
Mixture Formation: Dispersed Phase

Detailed Simulation of Nozzle Influence on Atomization

Fully developed turbulent inflow

Actual nozzle inflow

Le Chenadec, V., Pitsch, H., "A conservative framework for primary atomization computation and application to the study of nozzle and density ratio effects", Atomization and Spray, 23, 2013
Detailed Simulation of Spray A case (ECN) with exact geometry

- Reynolds number 60,000
- Weber number 1,100,000
- LES done with 242 Mio. Cells
  - no-slip BC
  - exact geometry
  - low-Mach
- Primary Breakup Simulations to be done

1. CMT: ECN workshop 3, Modeling Presentation, 2014
Mixture Formation: GDI

Detailed Simulation of Nozzle Influence on Atomization (GDI)

(Content removed)
Mixture Formation

Using PB Results as Boundary Condition for Lagrange Simulation

- Combined primary breakup and Lagrange spray (CPBLS)
- Tuned Fully-Lagrange spray (FLS)

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Mixture Formation

Using PB Results as Boundary Condition for Lagrange Simulation

- FLS DSD shifted to large droplet sizes at 30 mm downstream
- FLS DSD shifted to smaller droplet sizes at 70 mm downstream
- CPBLS DSD in good agreement with experiments everywhere

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Combustion Chemistry

- Chemical kinetics combustion
  - Auto-ignition
  - Pollutant formation

- Advanced engine combustion processes are kinetically controlled

- Definition of surrogates for real fuels
n-Dodecane Model Development

Species profiles

Ignition delay times

Laminar flame speeds

n-Dodecane Model Reduction

- **Automatic reduction**
  - Directed Relation Graph with Error Propagation (DRGEP)
  - Species lumping

- ~80% Reduction
  - Detailed (*dotted line*): 294 species
  - Skeletal (*dashed line*): 207 species
  - Reduced (*solid line*): 63 species
n-Dodecane Model Optimization

- **Automatic optimization**
  - Method of Uncertainty Minimization using Polynomial Chaos Expansions (MUM-PCE)
  - Bayesian method

- **Improved model performance**
  - Detailed (*dotted line*)
  - Reduced (*dashed line*)
  - Optimized (*solid line*)
Representative Interactive Flamelet (RIF) Model

• Representative Interactive Flamelet model
  – Originally: Combustion model for diesel engine combustion
  – Extended to other internal combustion engine combustion modes
    → Auto-ignition
  – Extended to the bigger class of unsteady flamelet models

• Basic idea
  – Solve unsteady flamelet equations
    \[ \rho \frac{\partial Y_i}{\partial \tau} - \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} - \dot{m}_i = 0 \]
  – One or more flamelets, each representative for certain part of the integration domain
  – Parameters conditionally averaged over represented region
    • Scalar dissipation rate
  – Flamelet solutions provide species mass fractions as function of mixture fraction
  – Ensemble averaged quantities with presumed pdf
Representative Interactive Flamelet (RIF) Model

\[ \bar{Y}_i(\vec{x}) = \int_0^1 \bar{P}(Z)Y_i(Z)\,dZ \]

\[ \tilde{h}(\vec{x}) = \sum h_i(\bar{T})\bar{Y}_i(\vec{x}) \]

\[ \bar{x}_{st}, \bar{p}, \tilde{h} \]

\[ \bar{T}(\vec{x}), \bar{c}_p(\vec{x}) \]

\[ Y_i(Z) \]

\[ \text{Flamelet Code} \]
Simulation Framework

Interfacial flow simulation

Lagrangian approach

RIF w/ 245 species
Results for ECN Spray A Constant Volume Chamber

Inert Spray Calculations

• Generally good agreement

• Vapor penetration length slightly overestimated

• Liquid penetration length matches quite well

Experimental data by:
Results for ECN Spray A Constant Volume Chamber

Reactive Spray Calculations

- Ignition delay too long in the simulation
  - 0.39 ms (exp) vs. 0.52 ms (sim)
- Vapor penetration length and shape of the flame looks quite well

Experimental data by:

Results for ECN Spray A Constant Volume Chamber

Reactive Spray Calculations – Emission Formation

• Reaction mechanism includes NO\textsubscript{X} formation pathways

• Soot formation is considered using HMOM model

Experimental data by:

Future Outlook

- High fidelity models important
- Importance of validation
- Engine experiments too complex
- DNS will be important

DNS of Igniting Diesel Spray

\[ t = 0.48 \quad t = 0.5 \]
Thank you for your attention!

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