LCRC Project: cfd_enginemodeling

Project Title: Computation Fluid Dynamics Modeling of Petrodiesel and Biodiesel

Project URL: (optional)

Select Division: Energy Systems

Select PIs and Members: Sibendu Som, Douglas E. Longman

Funding Source: LDRD Strategic Initiative (Integrated Bio-fuel/Engine Design), DOE Vehicle Technologies Program Office, Caterpillar Inc.

Abstract: Combustion and emission characteristics of compression ignition engines depend strongly on inner-nozzle flow and spray behavior. These processes control the fuel-air mixing, which in turn is critical for combustion processes. Our previous studies have highlighted the differences in the physical and chemical properties of petrodiesel and biodiesel, which significantly altered the inner-nozzle flow and spray structure. In this work, we aim to gain fundamental understanding of the influence of fuel properties on the combustion and emission characteristics of the compression ignition engine. N-heptane and methyl butanoate were selected as surrogates for diesel and biodiesel fuel respectively, since the chemical-kinetic pathways are well understood. Detailed spray models for atomization and breakup, drag, collision and coalescence, in addition to evaporation, combustion, and emission models were used. Full-cycle diesel engine simulations were performed for validation against motoring and combusting data from Caterpillar single-cylinder engine at 371 high-bay. More fundamental studies focused on establishing the mechanism for flame stabilization by estimating turbulent burning velocity for both the fuels. Extensive validation was performed against non-evaporating spray data obtained from x-ray radiography experiments at APS. Validation of the detailed chemistry approach was also performed by comparison of flame lift-off length data from University of Illinois at Urbana Champaign. All these studies were performed using the software, CONVERGE.

New Results: A tertiary component mixture of Methyl Decanoate (MD), Methyl-9-Decenoate (MD9D), and n-heptane (NHPT) was used as a surrogate for soy-derived biodiesel. The detailed mechanism consisted of 89 species and 364 reactions. The simulations were clearly able to predict the flame lift-off length, equivalence ratio values, and soot distribution.

The instantaneous experimental images obtained using Rayleigh scattering are shown on the left along with the time after start of injection and the axial length scale (see attached Figure). Both RANS and LES simulations predict the dispersion and vapor penetration fairly well. *However, marked differences in the spray structure are clearly observed between RANS and LES cases. While RANS predicts smooth, averaged profiles, the LES simulation is able to capture the instantaneous structure well*.

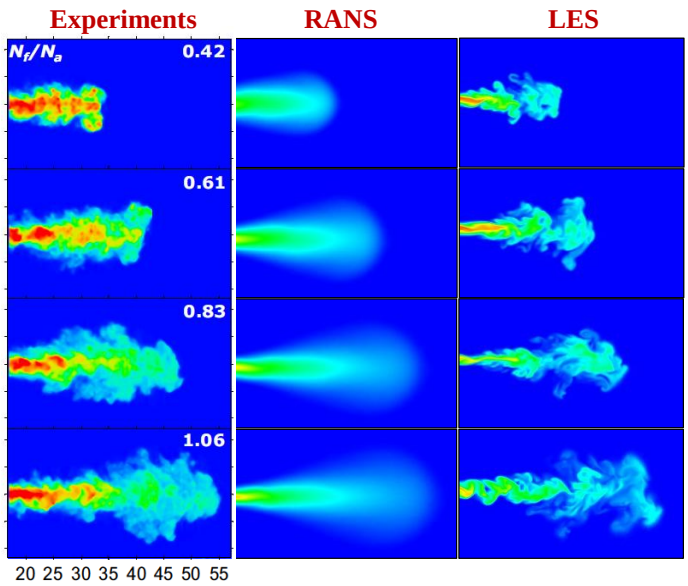

Figure 1: Images comparing the instantaneous equivalence ratio calculated using RANS and LES models, respectively, with experimental data from Sandia National Laboratory under non-reacting conditions.

Project Impact:

1) The KH-ACT model facilitates coupling of nozzle flow with spray and combustion simulations. The industry has been hampered in the past two decades due to the absence of a primary breakup spray model which can account for nozzle flow effects such as cavitation and turbulence. The KH-ACT model also captures the influence of fuel property differences between diesel and biodiesel fuels. Currently, this model is being implemented in the proprietary codes of Caterpillar Inc., Ford, CSI, and University of Wisconsin at Madison.
   http://www.transportation.anl.gov/engines/multi_dim_model_fuel_spray.html
2) The LES turbulence model has shed further insights into the flame stabilization mechanism. Also, both qualitatively and quantitatively the LES model seems to better predict combustion characteristics than RANS (Reynolds Averaged Navier Stokes) based models.
   http://www.transportation.anl.gov/engines/multi_dim_model_les.html
3) In the past, the use of reduced/simplified chemical kinetic mechanism which operated in a small equivalence ratio, temperature, and pressure regime severely hampered predictive capability of reacting flow codes for internal combustion engine (ICE) applications. Detailed chemical kinetic mechanisms developed in collaboration with UConn for diesel and biodiesel fuels has improved combustion predictions such as ignition delay, flame lift-off length, equivalence ratio, soot distribution etc.
   http://www.transportation.anl.gov/engines/multi_dim_model_combustion.html

New Capabilities:

Implementation and testing of new physical models:

1) Developed and implemented KH-ACT (Kelvin Helmholtz- Aerodynamics Cavitation Turbulence) primary breakup spray model
2) Robust validation of Smagorinsky based LES (Large Eddy Simulation) turbulence model in Converge software in collaboration with Convergent Science Inc. (CSI)
3) Developed and incorporated detailed chemical kinetic mechanism for diesel and biodiesel fuels in collaboration with University of Connecticut (UConn)

Scaling Studies: Scalability and Computational Efficiency for a high-fidelity spray-combustion simulation using detailed chemistry and LES turbulence model were conducted. Good scaling was seen up to 8 nodes for the problems studied.

Images: Attach Figure 1 (shown above).

Publications (Journal publications or book chapters your research has produced that relate to your LCRC computations):

1) S. Som, D.E. Longman, "Numerical study comparing the combustion and emission characteristics of biodiesel to petrodiesel," *Energy and Fuels* 25: 1373-1386, 2011.
2) S. Som, A.I. Ramirez, D.E. Longman, S.K. Aggarwal, "Effect of nozzle orifice geometry on spray, combustion, and emission characteristics under diesel engines conditions," *Fuel* 90: 1267-1276, 2011.
3) Z. Luo, T. Lu, M.J. Maciaszek, S. Som, D.E. Longman, "A reduced mechanism for high temperature oxidation of biodiesel surrogates," *Energy and Fuels* 24: 6283-6293, 2010.
4) S. Som, D.E. Longman, A.I. Ramirez, S.K. Aggarwal, "A comparison of injector flow and spray characteristics of biodiesel with petrodiesel," *Fuel* 89: 4014-4024, 2010.

Presentations (conference presentations or invited talks that relate to your LCRC computations):
Invited Talks:

1) S. Som, D.E. Longman, "Development of Spray and Combustion Models for Biodiesel from Different Feedstocks," *Presentation to Convergent Science Inc.*, Middleton *(WI, USA)*, August 4th 2011
2) S. Som, D.E. Longman, "Development of Spray and Combustion Models for Drop-in Biofuels," *Chemical Science and Engineering Division Seminar*, Argonne (IL, USA), July 6th 2011
3) S. Som, D.E. Longman, "Modeling and simulation capabilities at Argonne for ICE applications – Part 1," *Presentation to FORD modeling team*, Argonne (IL,USA), June 30th 2011
4) S. Som, D.E. Longman, "Modeling and simulation capabilities at Argonne for ICE applications – Part 2," *Presentation to FORD-Research and Innovation Center*, Dearborn (MI, USA), June 22nd 2011

Conference Presentations:

1) S. Som, D.E. Longman, Z. Luo, M. Plomer, T. Lu, P.K. Senecal, E. Pomraning, "Simulating flame lift-off characteristics of diesel and biodiesel fuels using detailed chemical-kinetic mechanisms and LES turbulence model," ICEF2011-60051, *ASME Internal Combustion Engine Division Fall Technical Conference*, Morgantown, October 2011.
2) S. Som, D.E. Longman, "Nozzle flow characterization of alternate fuels for compression ignition engine applications," *2011 SAE World Congress* (Presentation Only), Detroit, April 2011.
3) S. Som, D.E. Longman, Z. Luo, T. Lu, "Modeling Biodiesel Spray Flame lift-off and emission characteristics using a new detailed mechanism for methyl butanoate as surrogate," *2011 SAE World Congress* (Presentation Only), Detroit, April 2011
4) T. Lu, M. Plomer, Z. Luo, S.M. Sarathy, W.J. Pitz, S. Som, D.E. Longman, "Directed Relation Graph with Expert Knowledge for Skeletal Mechanism Reduction," *7th US National Combustion Institute Meeting*, Atlanta, March 2011.
5) Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman, "A Reduced Mechanism for Biodiesel Surrogates with Low Temperature Chemistry," *7th US National Combustion Institute Meeting*, Atlanta, March 2011.
6) Z. Lou, T. Lu, S. Som, D.E. Longman. Numerical Study on Combustion Characteristics of Biodiesel Using A New Reduced Mechanism for Methyl Decanoate as Surrogate (ICEF2010-35198). *ASME Internal Combustion Engine Division Meeting Fall Technical Conference*, San Antonio, September 2010.

Other Presentations:

1) S. Som, "Compilation of Spray-A modeling efforts," *Engine Combustion Network Workshop-1,* Ventura, May 2011
2) S. Som, D.E. Longman, "Spray-Combustion modeling set-up at Argonne National Laboratory," *Engine Combustion Network Workshop-1,* Ventura, May 2011
3) S. Som, D.E. Longman, "Integrated nozzle flow, spray and combustion modeling using KH-ACT primary breakup model and detailed chemistry," *AEC/HCCI Working group meeting at Sandia National Laboratory*, Livermore, February 2011
4) S. Som, D.E. Longman. Incorporating Fundamental Fluid Dynamics and Combustion Chemistry into Diesel Engine Simulations. U of C Review of the Energy Engineering and Systems Analysis ALD, November 18-19, 2010.
5) S. Som, D.E. Longman. Integrated Nozzle flow, Spray, Combustion, and Emission Modeling Using KH-ACT Primary Breakup Model and Detailed Chemistry. 2010 Directions in Engine-Efficiency and Emission Research (DEER) Conference, September 27-30, 2010.
6) S. Som. A Comparison of Nozzle Flow and Combustion Characteristics of Biodiesel with Diesel for Engine Applications. Argonne Post-Doctoral Symposium, September 8, 2010.

Grants:

1) TSA with Caterpillar Inc. for incorporating KH-ACT model in proprietary code titled, "Implementation of Spray Breakup Model in Caterpillar Engine Modeling Software," February-September 2011.

2) LDRD - DCG titled, “Detailed and Reduced Chemical Kinetics of Green Fuels for Compression Ignition Engine Modeling,” FY 2011-12.
3) TSA with Caterpillar Inc. titled, “Simulation of Internal Combustion Engines with High-Performance Computing tools,” FY 2011-12.