Argonne's KH-ACT Model

Incorporating Fundamental Fluid Dynamics and Detailed Combustion Chemistry into Diesel Engine Simulations

Sibendu Som, Energy Systems Division

Opportunity

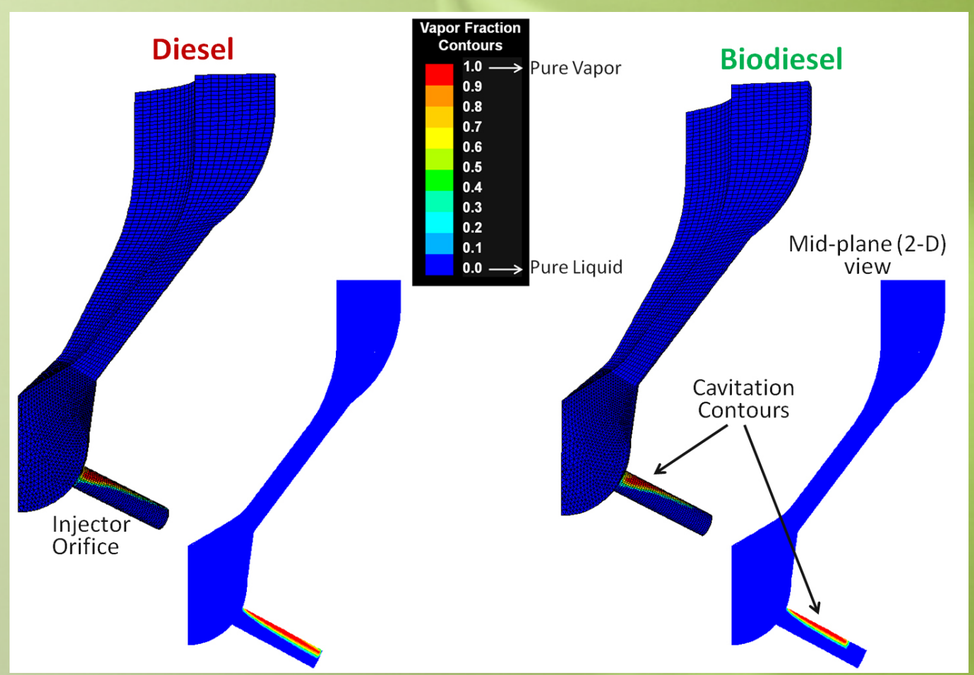
Biodiesel is a promising renewable biofuel due to its compatibility with the current diesel fuel infrastructure. Incorporating biodiesel into the existing infrastructure can be greatly expedited using computational modeling tools.

However, the spray atomization models that are currently used in diesel engine simulations generally consider aerodynamically induced breakup using the Kelvin-Helmholtz (KH) instability model, but do not account for in-nozzle flow effects.

In addition, surrogate mixtures for diesel and biodiesel fuels, and their chemical kinetics of combustion, are not well established.

Solution

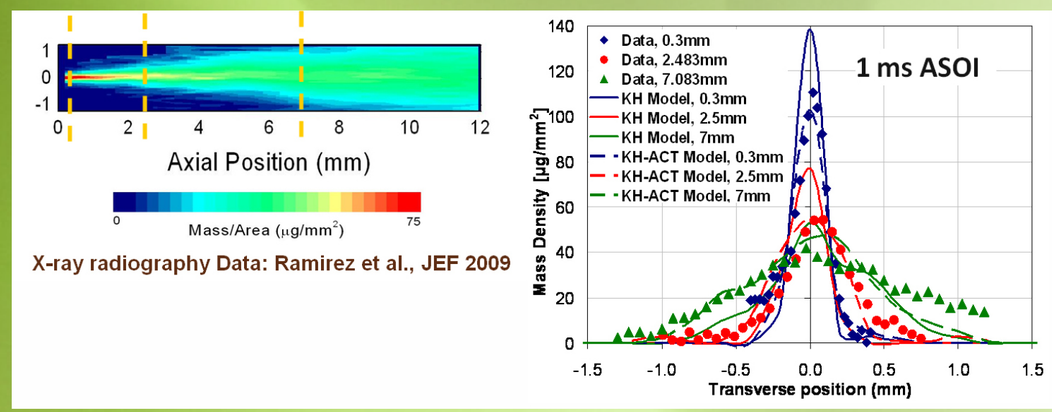
Argonne researchers helped develop an improved primary breakup model that integrates the effects of nozzle flow. The Kelvin-Helmholtz-Aerodynamics Cavitation Turbulence (KH-ACT) model considers cavitation and turbulence effects along with aerodynamically induced breakup, providing the ability to capture the influence of in-nozzle flow and fuel properties on spray, combustion, and emission processes.



What We've Achieved

Extensive validation of the KH-ACT model was performed against X-ray radiography data from Argonne. Under the conditions investigated, the enhanced primary breakup model is observed to provide better predictions for spray penetration and dispersion, as well as liquid and lift-off lengths.

Argonne researchers also quantified the influence of biodiesel on nozzle flow, spray, combustion and emission processes, and compared the results with petrodiesel.



Detailed chemical-kinetic models for biodiesel are developed in collaboration with University of Connecticut using directed relation graph, isomer lumping, and sensitivity analysis methods.

Benefits

- The expense of experimental research may be reduced by the integration of nozzle flow, spray, combustion, and emission modeling.
- Disparities in viscosity, vapor pressure, and density have revealed important differences in nozzle flow characteristics for diesel and biodiesel, which influence spray and combustion behavior.
- Fundamental (detailed) chemical-kinetics information provides further insights into the combustion process.

Future Work

- Incorporate improved turbulence models
- Perform full-cycle diesel engine simulations
- Parametric studies:
  - Effect of biodiesel feedstock variability
  - Effect of nozzle-orifice geometry and surface finish

Funding is provided by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Program, and Argonne's Integrated Biofuel/Engine Design LDRD Strategic Initiative. Collaborators include the University of Illinois at Chicago, the University of Connecticut, and Caterpillar, Inc. Supporting research was conducted at Argonne's Advanced Photon Source and the Laboratory Computing Resource Center.

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