LA-LP 10-017

Licensable Technologies

KIVA—Hydrodynamics Model for Chemically Reacting Flow with Spray

Applications:

- Flow and combustion modeling in spark-ignition, diesel engines, and gas turbines
- Analysis of flows in automotive catalytic converters
- Design of fire suppression systems
- Pulsed detonation propulsion systems design

Benefits:

- Increases engine efficiency while reducing harmful by-products
- Reduces engine development time

Contact:

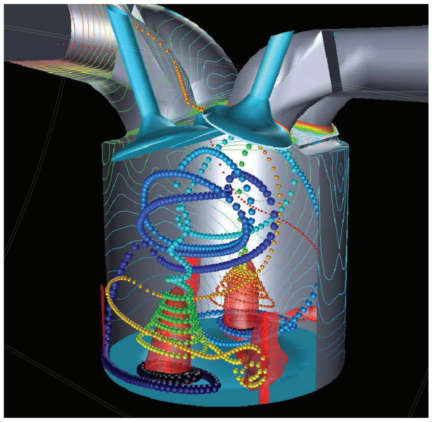
Doruk Aytulu
(505) 667-5315
doruk@lanl.gov

tmt-4@lanl.gov

Technology Transfer Division

Summary:

Fuel economy is heavily dependent upon engine efficiency, which in turn depends to a large degree on how fuel is burned within the cylinders of the engine. Higher in-cylinder pressures and temperatures lead to increased fuel economy, but they also create more difficulty in controlling the combustion process. Poorly controlled and incomplete combustion can cause higher levels of emissions and lower engine efficiencies.



Simulation of an experimental engine with DOHC quasi-symmetric pent-roof combustion chamber and 4 valves.

In order to optimize combustion processes, engine designers have traditionally undertaken manual engine modifications, conducted testing, and analyzed the results. This iterative process is painstakingly slow, costly, and does not lend itself to identifying the optimal engine design specifications. In response to these problems, Los Alamos National Laboratory (LANL) scientists have developed KIVA, an advanced computational fluid dynamics (CFD) modeling code that accurately simulates the in-cylinder processes of engines.

KIVA, a transient, three-dimensional, multiphase, multicomponent code for the analysis of chemically reacting flows with sprays has been under development at LANL for several years. The code uses an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite-volume technique. The code uses an implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving manner. Also, the convection calculations can be subcycled in the desired regions to avoid restricting the time step due to Courant conditions.

KIVA's functionality extends from low speeds to supersonic flows for both laminar and turbulent regimes. Transport and chemical reactions for an arbitrary number of species and their chemical reactions is provided. A stochastic particle method is used to calculate evaporating liquid sprays, including the effects of droplet collisions, agglomeration, and aerodynamic breakups.

Although specifically designed for simulating internal combustion engines, the modularity of the code facilitates easy modifications for solving a variety of hydrodynamics problems involving chemical reactions. The versatility and range of features have made KIVA programs attractive to a variety of non-engine applications as well. These range from convection towers to modeling silicon dioxide condensation in high pressure oxidation chambers. Other applications have included the analysis of flows in automotive catalytic converters, power plant smokestack cleaning, pyrolytic treatment of biomass, design of fire suppression systems, pulsed detonation propulsion systems, stationary burners, aerosol dispersion, and design of heating, ventilation, and air conditioning systems. The code has found a widespread application in the automotive industry.

Recently, LANL researchers developed KIVA-4mpi, a parallel version of KIVA-4. This software also solves chemically reacting, turbulent, multi-phase viscous flows, but does this on multiple computer processors with a distributed computational domain (grid). KIVA-4mpi internal engine combustion modeling capabilities are the same as that of KIVA-4, and are based on the KIVA-4 unstructured grid code.

Development Stage: General availability

Intellectual Property Status: Multiple copyrights

Licensing Status: Available for non-exclusive licensing

Los Alamos NATIONAL LABORATORY ESTABLISHED 1943

4/12