KIVA Modeling to Support Diesel Combustion Research

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Acknowledgements: Dan Flowers and Tom Piggott of LLNL

This presentation does not contain any proprietary or confidential information.
• KIVA-4 allows one to simulate internal combustion engines with the goal of improving efficiency and reducing emissions.
  – Open source (incentive for submodel development).
• Parallel computations and unstructured geometries can be accommodated.
• KIVA-4 has been interfaced with existing combustion capabilities (Lawrence Livermore’s Multi-zone model and the University of Wisconsin’s Engine Research Center (UW-ERC) model) to increase its applicability to a variety of engine simulations.
• Parallel Large Eddy Simulation (LES) turbulence capability has been implemented in KIVA-4.
Recommendations from 2007 Merit Review

• Encouraged to develop more industry interaction.
• Are there mechanisms in place to take some of the code developments to other CFD codes?
• Interesting, detailed work, but the wrap around to experimental work was not obvious.
• Use more realistic geometry for validation. Should have more focus on 4 valve engines.
• Barriers involve integration of other models into KIVA-4 and comparison with experimental data.
• Approach is to interface combustion models (multi-zone, ERC, LES) with KIVA-4 and integrate experimental comparisons through collaboration.
Accomplishments

- Parallel KIVA-4 LES turbulence
- Parallel KIVA-4 Multi-zone
  - In collaboration with Dan Flowers and Tom Piggott of LLNL
- KIVA-4 University of Wisconsin Engine Research Center (UW-ERC) model testing by Iowa State University
- New geometries
- Reducing the spray dependence with overset method
Why? In an engine, all length scales cannot be resolved.

\[
\frac{\text{Largest length scale}}{\text{Smallest length scale}} \mu \text{Re}^{3/4} \quad \text{Re} = \frac{\Box U L}{\Box}
\]

\(\Box = \text{density}, \ U = \text{velocity}, \ L = \text{Largest length scale}, \ \Box = \text{viscosity}\)

- In 1D, the number of grid points \((N)\) required to resolve the smallest scale is
- \(N \Box (\text{Re}^{3/4})^3\) for a 3D mesh.

\(\text{Re} \approx 50000, \ \text{Re}^{9/4} = 37 \times 10^9\)
Turbulence models

- **RANS** (Reynolds-Averaged Navier-Stokes)
  - Temporal average.
  - All spatial scales are modeled or approximated.
- **LES** (Large Eddy Simulation)
  - Spatial average.
  - Large spatial scales are resolved and small scales (subgrid-scales) are modeled. Subgrid scales are more isotropic and universal.
  - Typically requires more resolution than RANS.
- **DNS** (Direct Numerical Simulation)
  - Attempt is made to resolve all scales.

\[
\overline{f}(x,t) = \frac{1}{T} \int_{t}^{t+T} f(x,t) \, dt
\]

\[
\overline{G}(x \cdot y) = \int_{V} G(x \cdot y) \, dy
\]

*Arrow shows the direction of increasing computational expense.*
LES Implementations


We will be looking at the Dynamic Structure Model in future KIVA-4 LES implementations.
Internal energy

\[
\frac{\partial \tilde{I}}{\partial t} + \tilde{\nabla} \cdot (\tilde{\nabla} \tilde{I}) = \tilde{p} \tilde{\nabla} \cdot \tilde{u} + A_o \tilde{\nabla}_L \cdot \tilde{u} \tilde{\nabla} \cdot \tilde{J} + W_T
\]

Turbulent kinetic energy

\[
\frac{\partial \tilde{k}}{\partial t} + \tilde{\nabla} \cdot (\tilde{\nabla} \tilde{k}) = \frac{2}{3} \tilde{\nabla} \tilde{k} \cdot \tilde{u} + \tilde{\nabla} : \tilde{\nabla} \tilde{u} + \tilde{\nabla} \cdot \left( \frac{\tilde{\nabla} \tilde{u}}{\text{Pr}_T} \right) \tilde{k} \tilde{\nabla} W_T
\]

\[W_T = \tilde{\nabla} A_0 = 0 \text{ in k-epsilon} \quad W_T = \frac{C_e \tilde{k}^2}{\text{Pr}_T}, \ A_0 = 1 \text{ in LES}\]

\[\text{Pr}_T = \tilde{\nabla} C_m \frac{k^2}{\text{Re}} \text{ in k-epsilon} \quad \text{Pr}_T = \tilde{\nabla} C_m \sqrt{k} \text{ in LES}\]

Turbulent viscosity affects mass diffusion and momentum.
Issues with LES

• Resolution of extremely fine spatial scales near the wall - law of the wall is currently used.
• Accuracy of the numerical scheme in complex geometries and its influence on LES turbulence.
• Spray and LES.
Comparison of k-epsilon and LES of fuel distribution

2 bar pressure inflow boundary
Intake port: \(0.11\) mass fraction iso-octane

Parallel 4-processor calculation in an unstructured hexahedral mesh with KIVA-4.

128K grid at BDC,
Initial conditions:
300K, 1 bar,
\(0.01\) mass fraction iso-octane
K-epsilon and LES show similarities in fuel distribution at 15 CAD. However differences in the turbulence models develop later in the simulation.
KIVA-4 Multi-zone

- Collaborative effort between Los Alamos and Lawrence Livermore.
- Lawrence Livermore’s multi-zone combustion model has been implemented in parallel KIVA-4 (Flowers, Aceves, Babajimopoulos, Assanis).
- The multi-zone model partitions cells into temperature and $F$ zones and solves the chemistry within each zone. This dramatically cuts down the computational time since the chemistry > 90% of computational time.
- The chemistry and the hydrodynamics are now parallelized in KIVA-4 MZ.
- Engine geometries can be run with unstructured meshes in KIVA-4 MZ.
KIVA-3 MZ

KIVA-4 MZ

Pressure KIVA-3 MZ
Pressure KIVA-4 MZ
Temperature KIVA-3 MZ
Temperature KIVA-4 MZ

Heat Release Rate (J/s)

CAD
KIVA-4 Enhancement for Diesel Engine Simulation

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Model Description

- Spray
- Ignition
- Combustion
Experimental Conditions

• Caterpillar 3401 engine
• High load, single injection
Results – CAT

- High load, double injection
Results – CAT

- Low load, single injection, PCCI conditions
New 3D engine geometries
Mesh constructed by Valmor de Almeida from Oak Ridge National Laboratory

Tetrahedral + Prism Mesh
Mesh contributed by J.Y. Chen of U.C. Berkeley
Reducing Spray Dependence

• Will be accomplished by the use of two grids - one for the spray particles and the other for the complex computational domain.

• Information will be mapped from one grid to the other.

• Issues have been addressed by many authors including Schmidt and Senecal, 2002, Abani et al. 2006, Beard et al. 2000, Stalsberg-Zarling 2005, Lippert et al. 2007.
Spray dependence issues

- **Evaporation**
  - When a parcel evaporates, all the evaporated mass is distributed throughout the cell the parcel resides within.

- **Momentum transfer**
  - When a parcel loses momentum through drag, the momentum transfer to the gas phase is linked to one node whose mass depends on the grid resolution.

- **Collisions**
  - Two parcels must reside within the same cell in order to collide.
Technology transfer

- Ford
  - Parallel validation and development of KIVA-4 in realistic engine geometries.
- Iowa State University
  - Testing of University of Wisconsin’s spray and combustion models in KIVA-4 using LANL’s initial implementation.
- Applied Research Laboratory at Penn State
  - Development of a spray model with reduced mesh dependence.
- Lawrence Livermore
  - Implementation of multi-zone model in KIVA-4
- Sandia National Laboratory
  - Paul Miles description of a non-linear turbulent stress model impact in KIVA-3V.
- Continue interactions with the University of Wisconsin, University of California at Berkeley and Oak Ridge National Laboratory.
Collaboration between Ford and Los Alamos

- Testing of piston-bowl geometries, 2-valve and 4-valve geometries with KIVA-4.
- Parallel testing of realistic valve geometries.
- Testing has improved the robustness of KIVA-4.


• Torres, D.J., Colocated KIVA-4, International Multidimensional Engine Modeling User’s Group Meeting at the SAE Congress (2007).


• Torres, D.J., KIVA-4: Validation, Rezoning and Remapping, 15th International Multidimensional Engine Modeling User’s Group Meeting at the SAE Congress (2005).

• Torres, D.J. and P.J. O'Rourke, KIVA-4, 14th International Multidimensional Engine Modeling User’s Group Meeting (2004).


Plans for Next Fiscal Year

- Continue LES turbulence model simulations in KIVIA-4 and implement the dynamic structure model.
- Continue to collaborate with Lawrence Livermore in applying the KIVA-4 multi-zone model to additional geometries.
Plans for Next Fiscal Year

- Test KIVA-4’s ERC models in other geometries in collaboration with Iowa State and the University of Wisconsin.
- Improve KIVA’s wall film model in collaboration with Iowa State.
- Apply grid overset method to sprays in more complex geometries.
- Continue validation (in parallel and with unstructured geometries).
• Implemented parallel KIVA-4 LES capability.
• Implemented KIVA-4 multi-zone capability in collaboration with Lawrence Livermore.
• Iowa State has tested KIVA-4’s UW-ERC models against experimental results (using LANL’s initial implementation of UW-ERC models into KIVA-4).
• Simulated spray using overset method in KIVA-4.