KIVA Modeling to Support Diesel Combustion Research

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Acknowledgements: Dan Flowers and Tom Piggott of LLNL

Purpose of work

- 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 and Approach

- 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

Turbulence Modeling

Why? In an engine, all length scales cannot be resolved.

$$\frac{Largest\ length\ scale}{Smallest\ length\ scale} \mu\ \mathrm{Re}^{3/4} \qquad \mathrm{Re} = \frac{\square UL}{\square}$$

$$\square = density, U = velocity, L = Largest\ length\ scale, \square = viscosity$$

- In 1D, the number of grid points (N) required to resolve the smallest scale is $\frac{Largest\ length\ scale}{Smallest\ length\ scale}$.
- N $\square$ $(\mathrm{Re}^{3/4})^3$ for a 3D mesh.

Re ≈50000, $\mathrm{Re}^{9/4} = 37\mathrm{x}10^9$

Turbulence models

- RANS (Reynolds -Averaged Navier-Stokes)
  - Temporal average.
  - All spatial scales are modeled or approximated.

$$\bar{\phi}(x,t) = \frac{1}{T}\int_{t}^{t+T} \phi(x,t)\,dt$$

- 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.

$$\bar{\phi}(x,t) = \int_{V} G(x - y)\,\phi(y,t)\,dy$$

- DNS (Direct Numerical Simulation)
  - Attempt is made to resolve all scales.

Arrow shows the direction of increasing computational expense.

LES Implementations

- Sone and Menon, Journal of Engineering for Gas Turbines and Power, 2003.
- Hori, Senda, Kuge and Fujimoto, SAE-2006-01-3334.
- Pomraning and Rutland, AIAA, 2002.
- Chumakov and Rutland, Int. Journal for Numerical Methods in Fluids, 2005.
- Huijnen, et al., Int. J. Num. Methods in Eng., 2005.

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

Differences in KIVA-4 k-epsilon and KIVA-4 LES

Internal energy

$$\frac{\partial \bar{\rho}\tilde{I}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\vec{u}}\tilde{I}) = -\bar{p}\nabla \cdot \tilde{\vec{u}} + A_o \bar{\sigma}_L : \nabla \tilde{\vec{u}} - \nabla \cdot \tilde{J} + W_T \qquad \tilde{\varepsilon} = \frac{\overline{\rho\varepsilon}}{\bar{\rho}}$$

Turbulent kinetic energy

$$\frac{\partial \bar{\rho} k}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\vec{u}}k) = -\frac{2}{3}\bar{\rho}k\nabla \cdot \tilde{\vec{u}} + \bar{\sigma} : \nabla \tilde{\vec{u}} + \nabla \cdot \left[\left(\frac{\mu_T}{\mathrm{Pr}_T}\right)\nabla k\right] - W_T$$

$$W_T = \bar{\rho}\tilde{\varepsilon},\ A_0 = 0 \ in\ k - epsilon \qquad W_T = \frac{C_\varepsilon \bar{\rho} k^{\frac{3}{2}}}{\Delta},\ A_0 = 1\ in\ LES$$

$$\mu_T = \bar{\rho} C_\mu \frac{k^2}{\tilde{\varepsilon}}\ in\ k - epsilon \qquad \mu_T = \bar{\rho} C_k \sqrt{k}\Delta\ in\ LES$$

Turbulent viscosity affects mass diffusion and momentum.

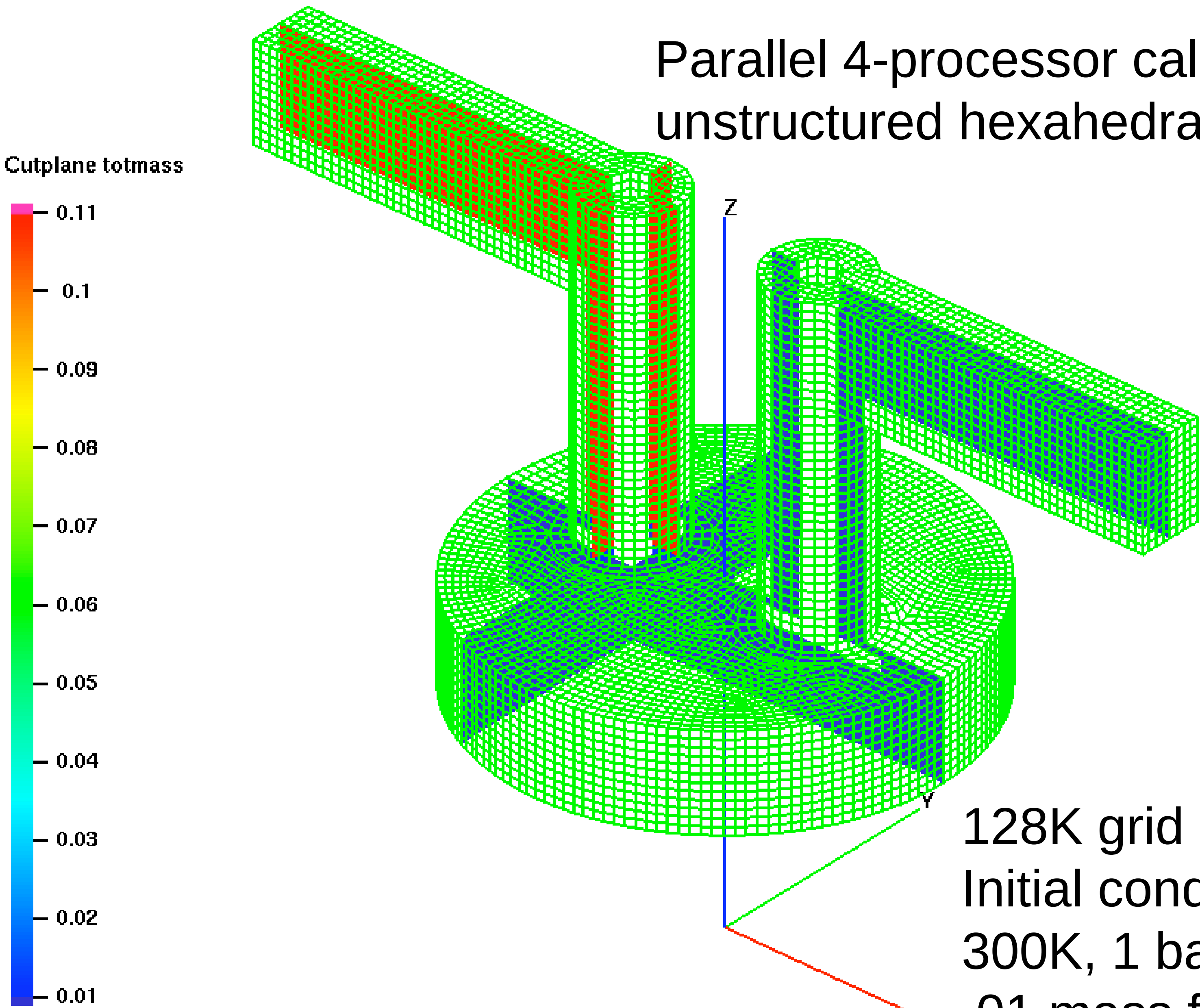
Issues with LES

- 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

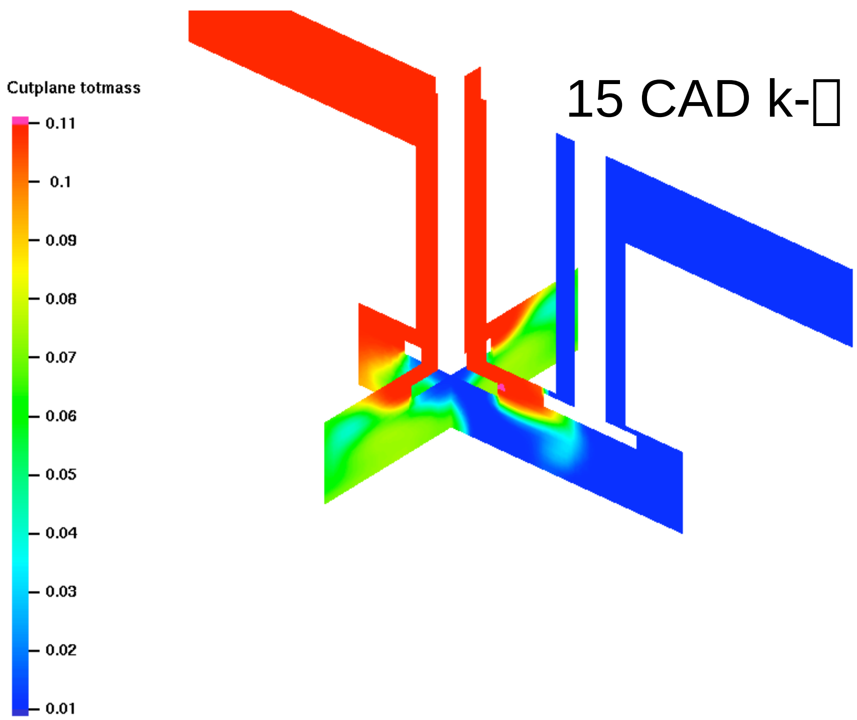
2 bar pressure inflow boundary
Intake port: .11 mass fraction iso-octane

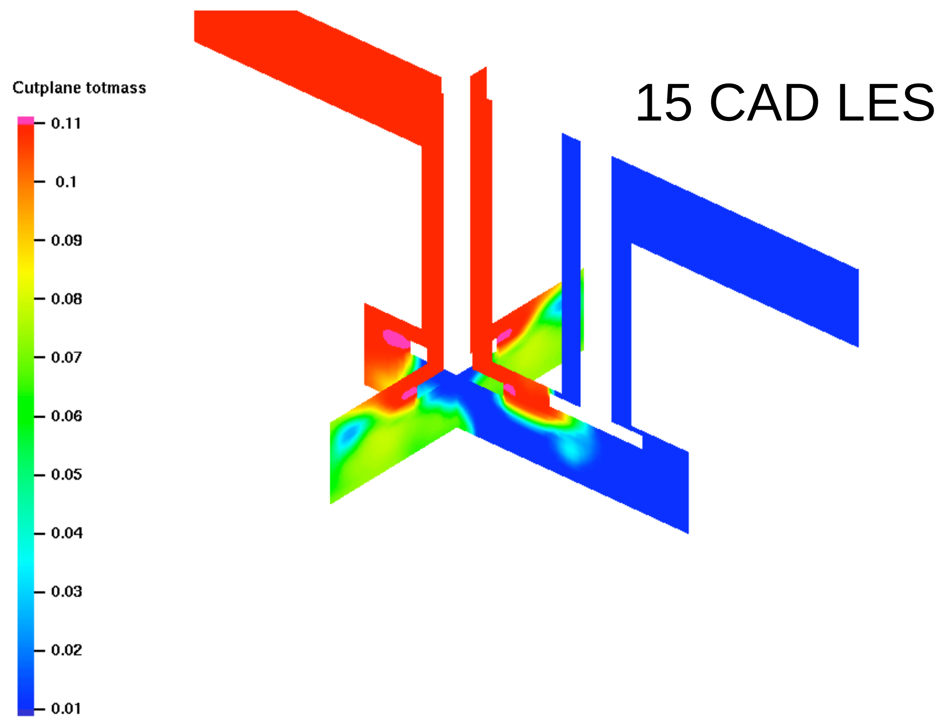
Parallel 4-processor calculation in an unstructured hexahedral mesh with KIVA-4.

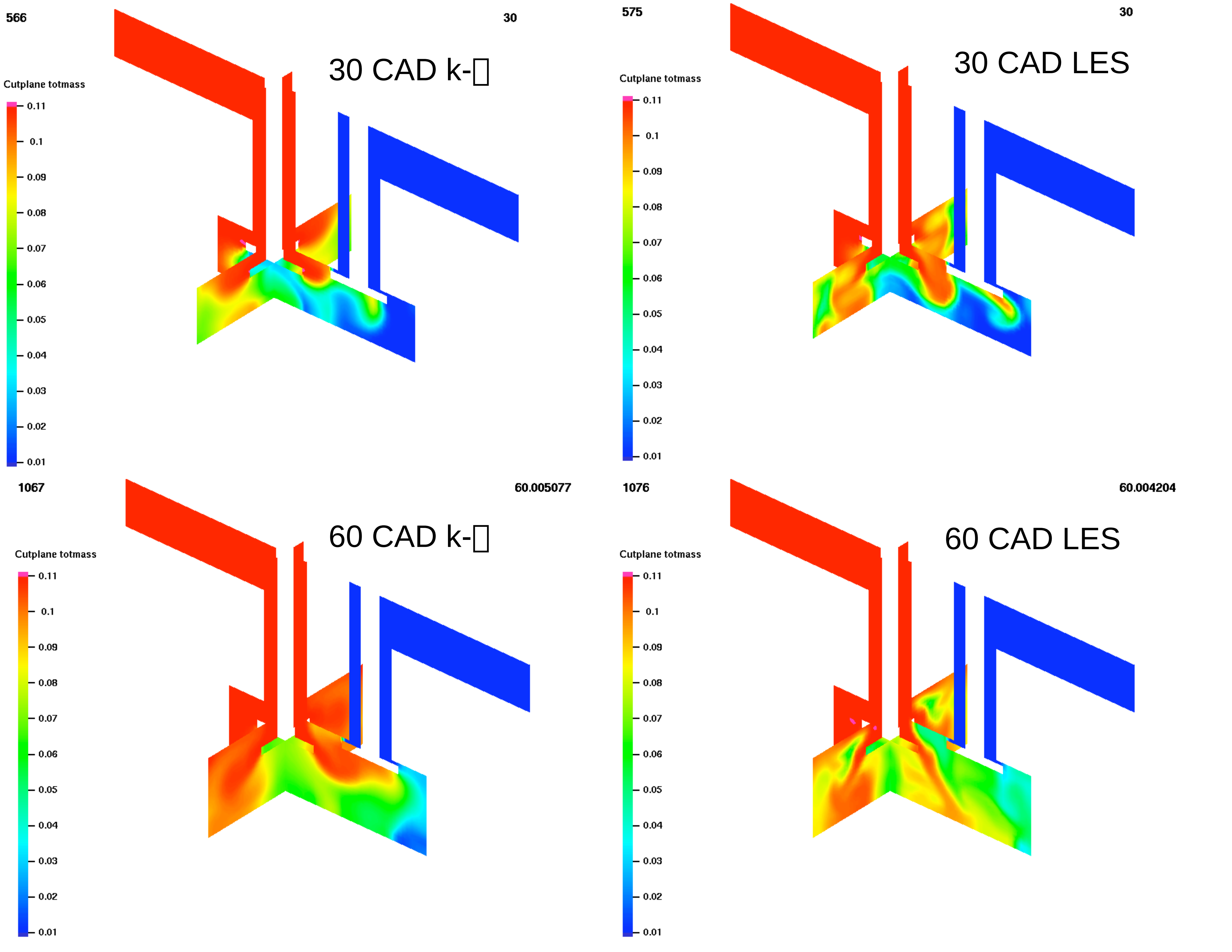


128K grid at BDC,
Initial conditions:
300K, 1 bar,
.01 mass fraction iso-octane

K-epsilon and LES show similarities in fuel distribution at 15 CAD. However differences in the turbulence models develop later in the simulation.



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30 CAD k-□
Cutplane totmass
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575
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30 CAD LES
Cutplane totmass
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0.03
0.02
0.01
1067
60.005077
60 CAD k-□
Cutplane totmass
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1076
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60 CAD LES
Cutplane totmass
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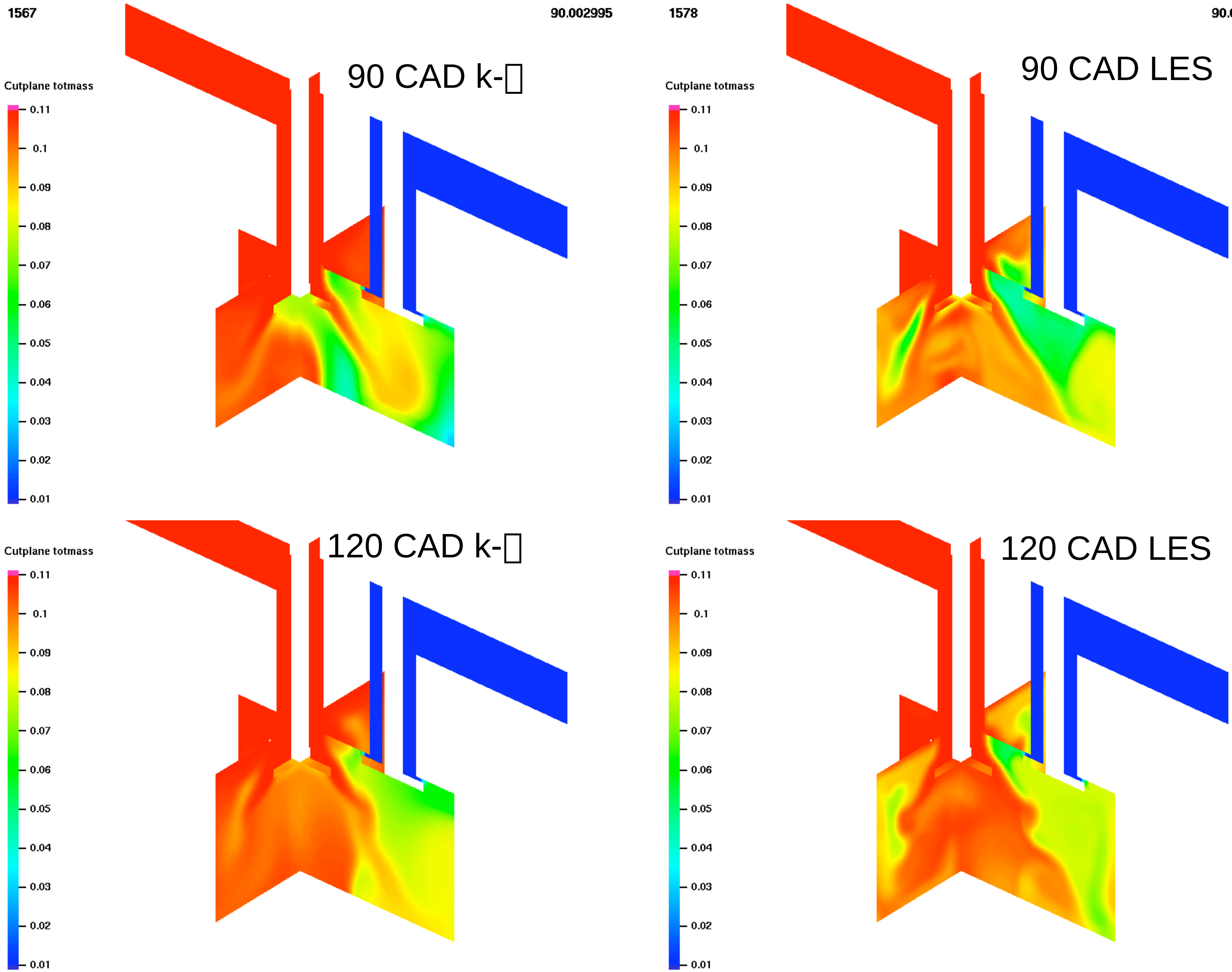

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90 CAD LES
Cutplane totmass
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0.01
120 CAD k-
Cutplane totmass
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120 CAD LES
Cutplane totmass
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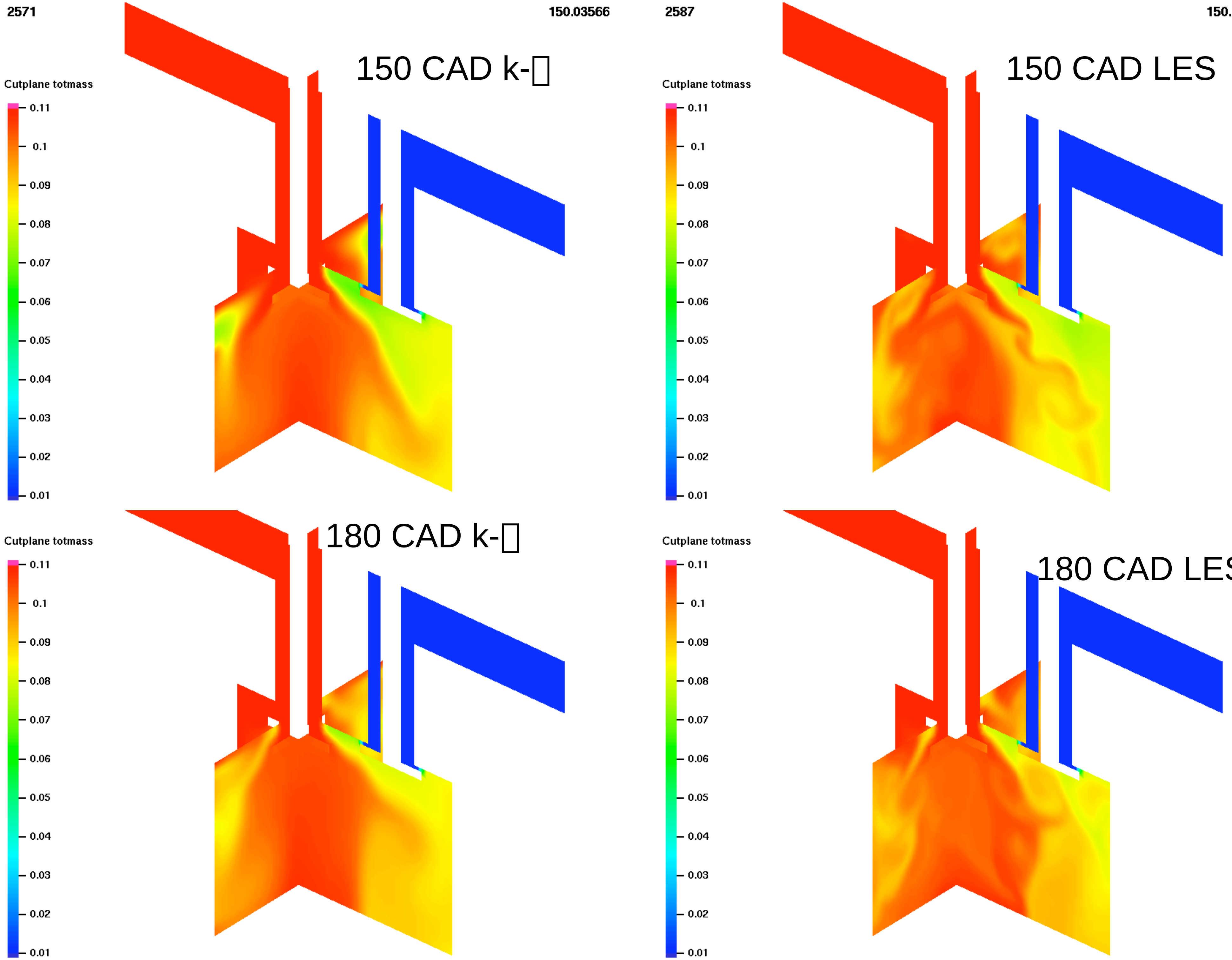
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0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
2587
150.
150 CAD LES
Cutplane totmass
0.11
0.1
0.09
0.08
0.07
0.06
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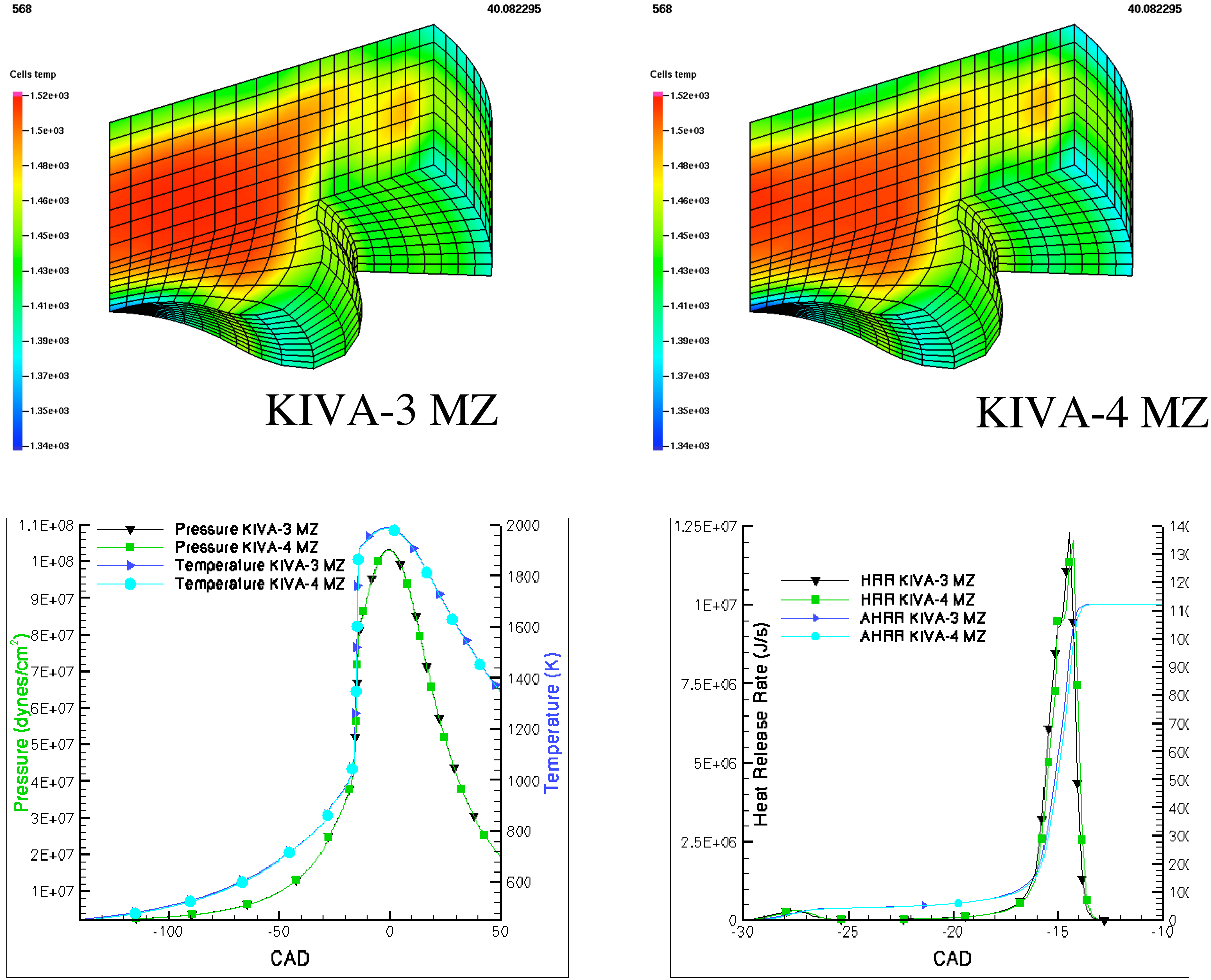
0.04
0.03
0.02
0.01
180 CAD k-
Cutplane totmass
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
180 CAD LES
Cutplane totmass
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01

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 □ 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.



568
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Cells temp
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1.5e+03
1.48e+03
1.46e+03
1.45e+03
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1.41e+03
1.39e+03
1.37e+03
1.35e+03
1.34e+03
KIVA-3 MZ
568
40.082295
Cells temp
1.52e+03
1.5e+03
1.48e+03
1.46e+03
1.45e+03
1.43e+03
1.41e+03
1.39e+03
1.37e+03
1.35e+03
1.34e+03
KIVA-4 MZ
Pressure KIVA-3 MZ
Pressure KIVA-4 MZ
Temperature KIVA-3 MZ
Temperature KIVA-4 MZ
Pressure (dynes/cm^2)
Temperature (K)
1.1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
2000
1800
1600
1400
1200
1000
800
600
-100
-50
0
50
CAD
HRR KIVA-3 MZ
HRR KIVA-4 MZ
AHRR KIVA-3 MZ
AHRR KIVA-4 MZ
Heat Release Rate (J/s)
1.25E+07
1E+07
7.5E+06
5E+06
2.5E+06
0
-30
-25
-20
-15
-10
CAD

KIVA-4 Enhancement for Diesel Engine Simulation

Song-Charng Kong
Department of Mechanical Engineering
Iowa State University

Model Description

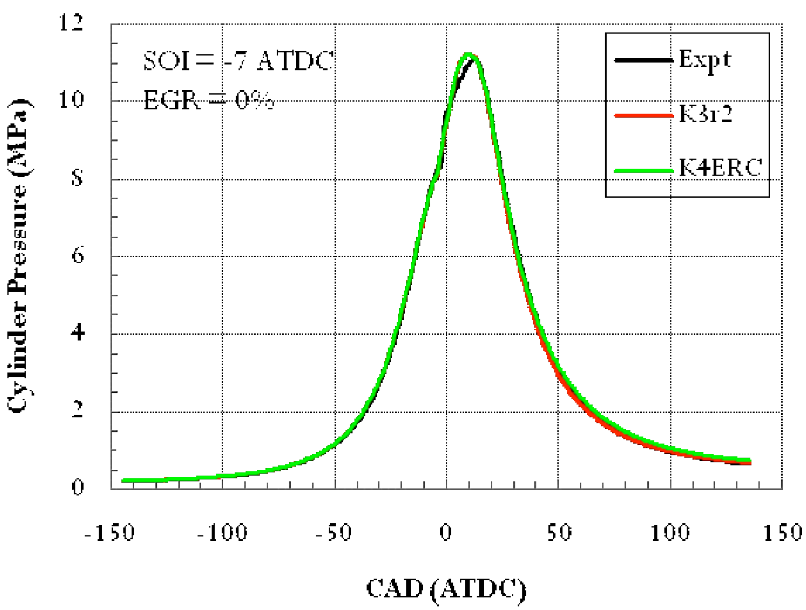
- Spray
- Ignition
- Combustion

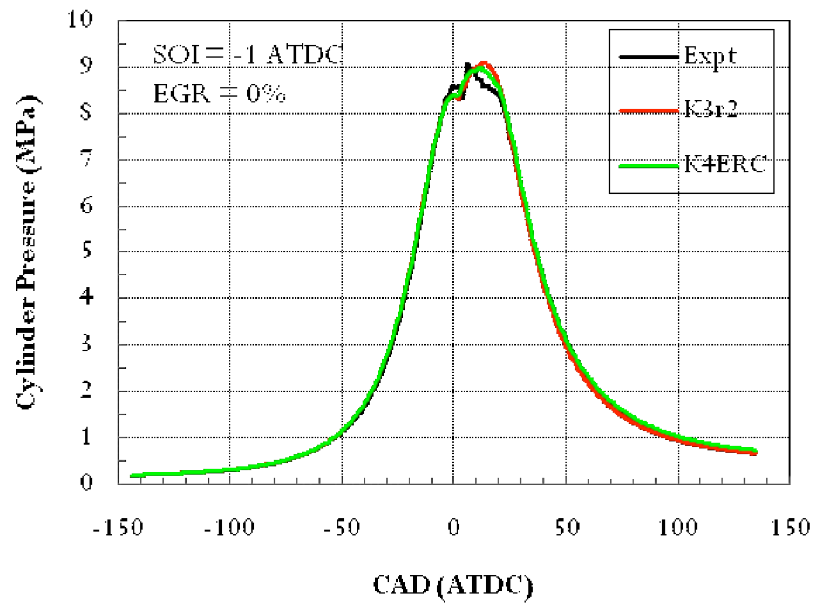
Experimental Conditions

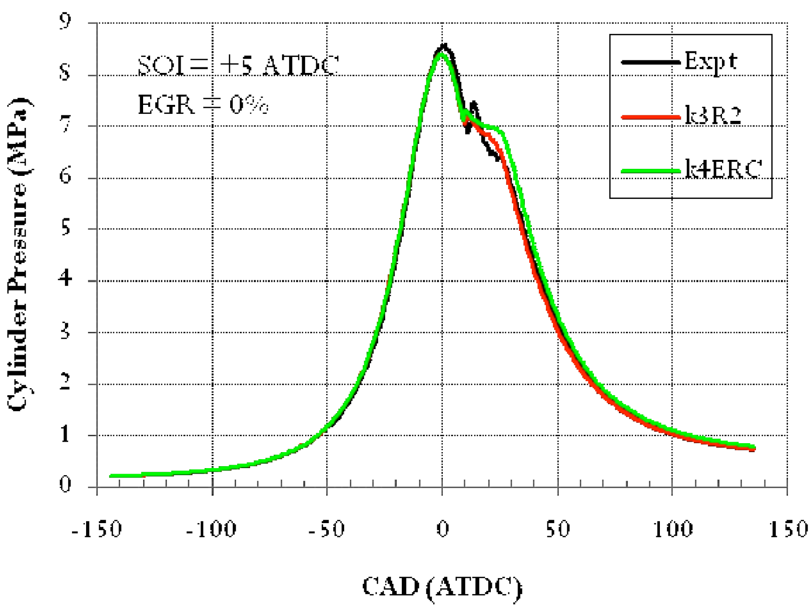
- Caterpillar 3401 engine

Results – CAT

- High load, single injection

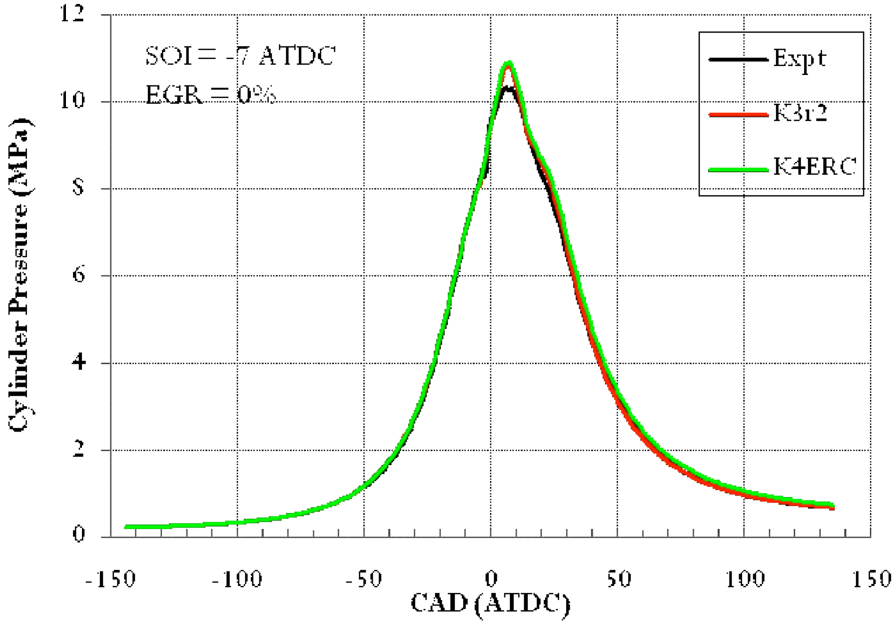


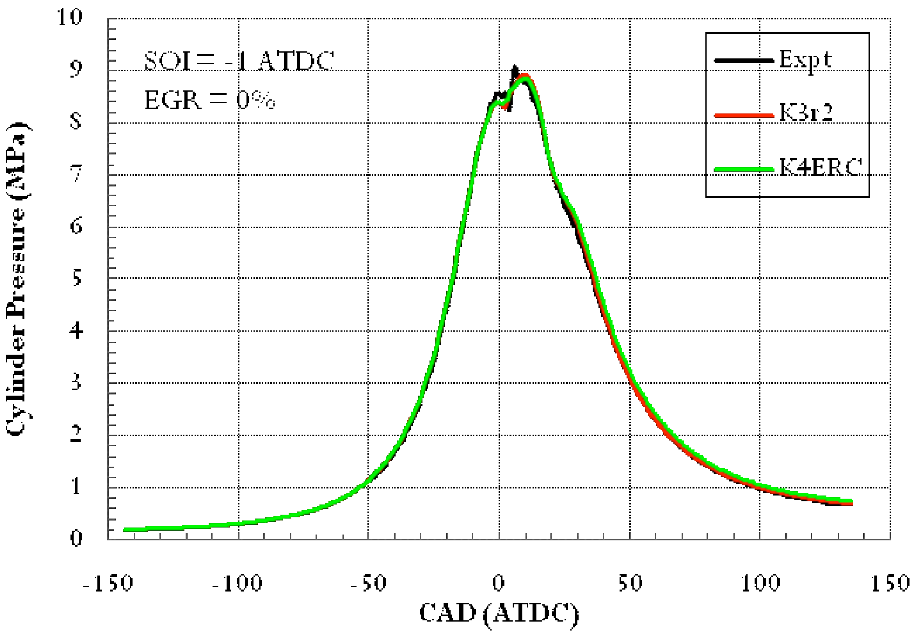


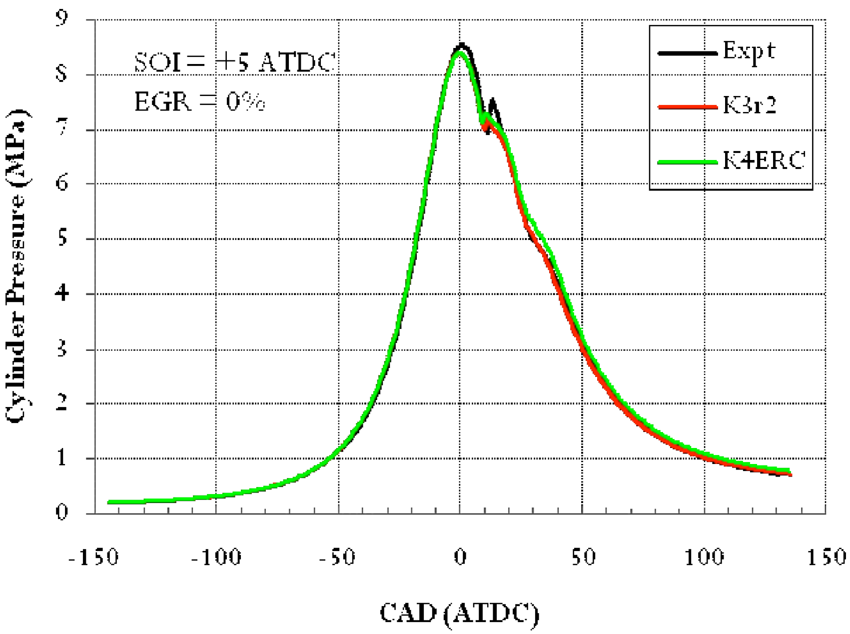


Results – CAT

- High load, double injection

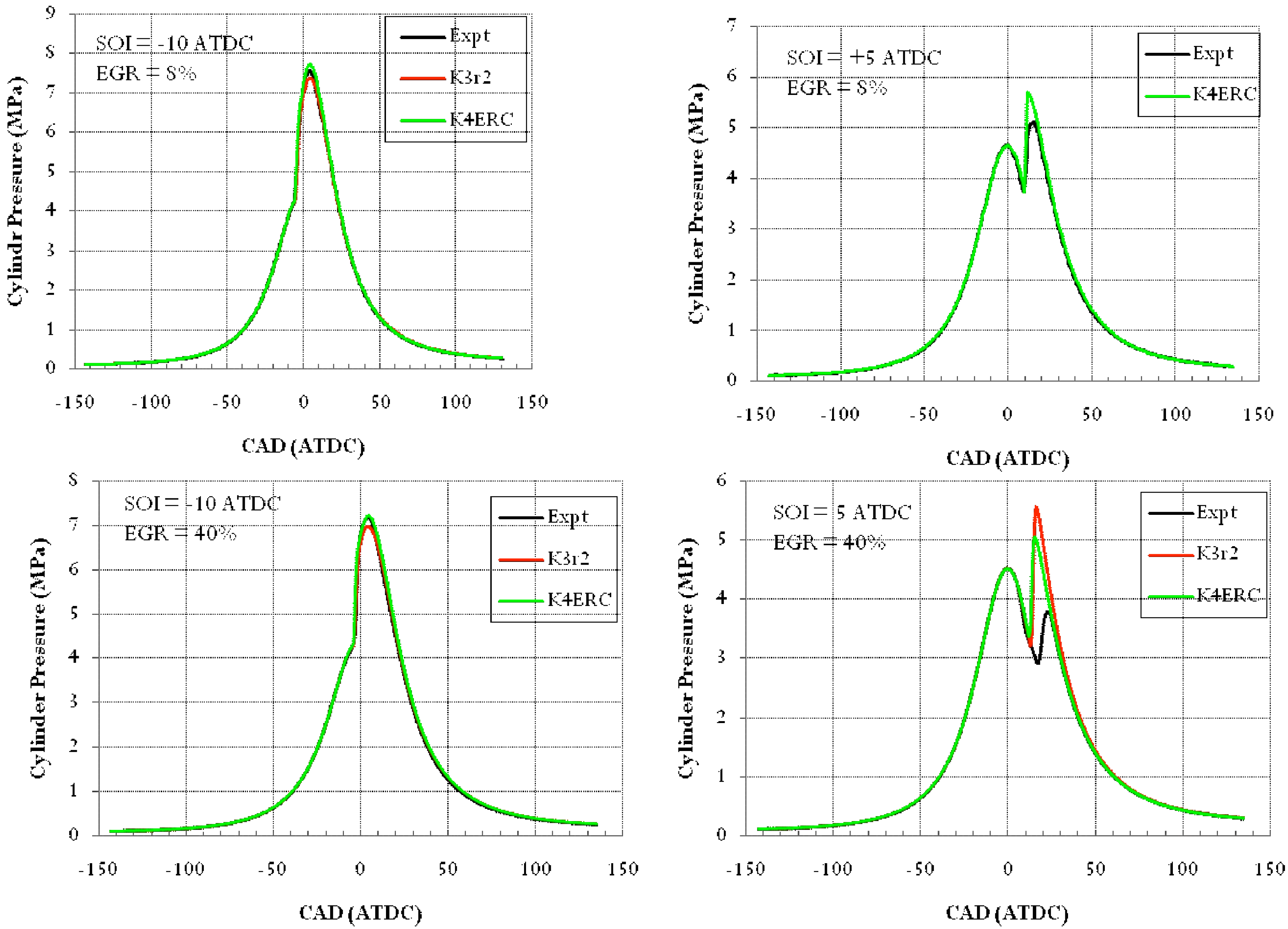




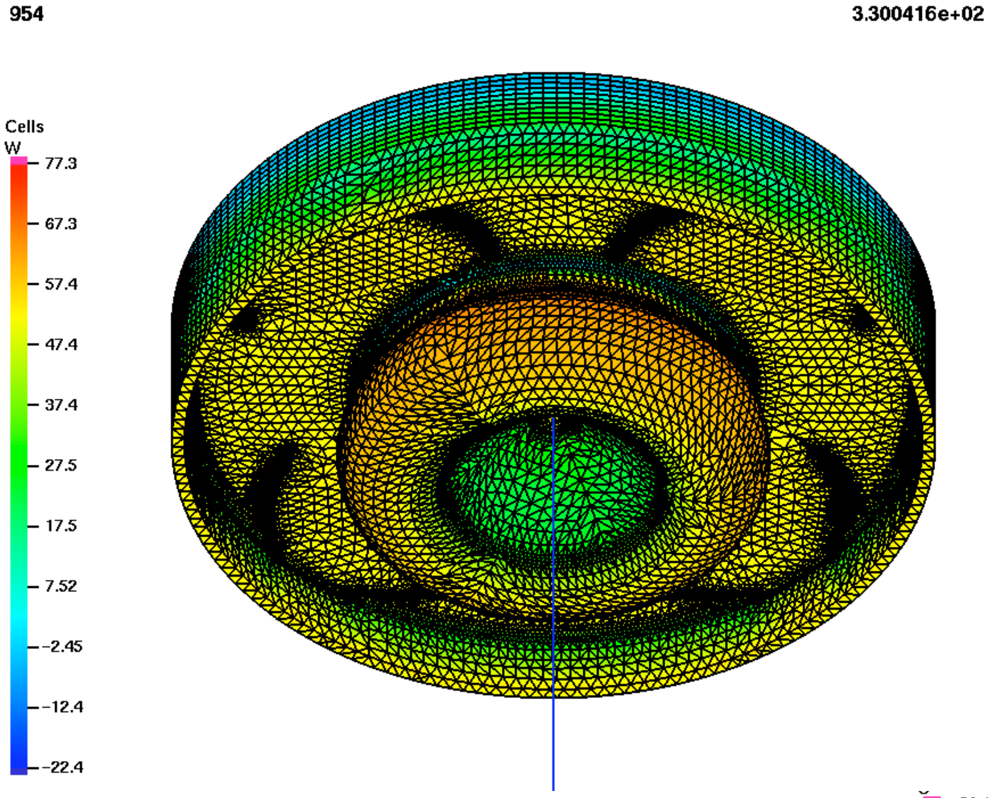


Results – CAT

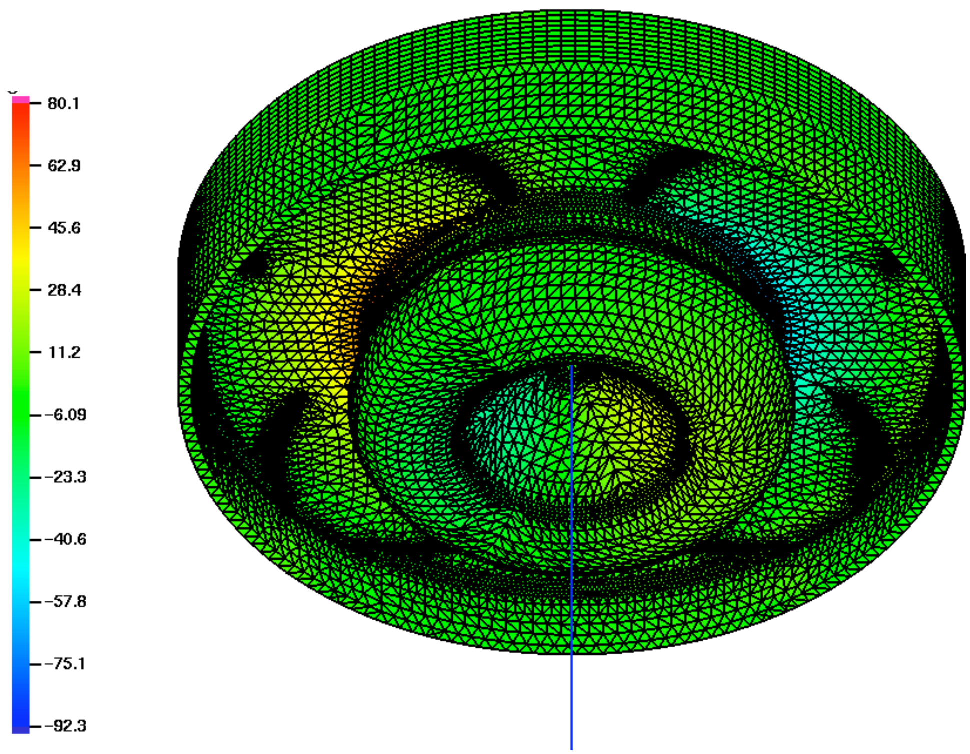
- Low load, single injection, PCCI conditions



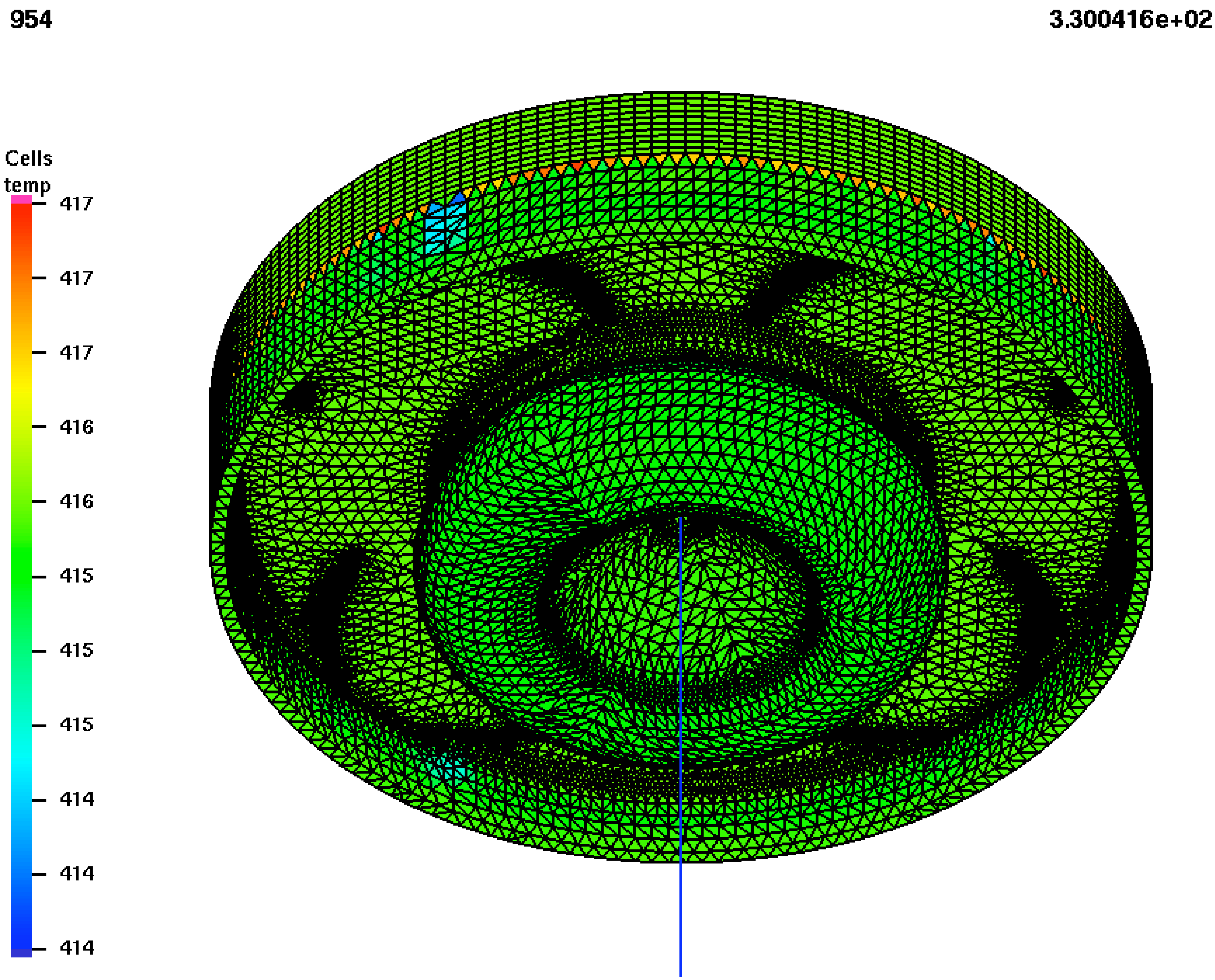
New 3D engine geometries



Mesh constructed by Valmor de Almeida from Oak Ridge National Laboratory



Tetrahedral + Prism Mesh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Cells
temp
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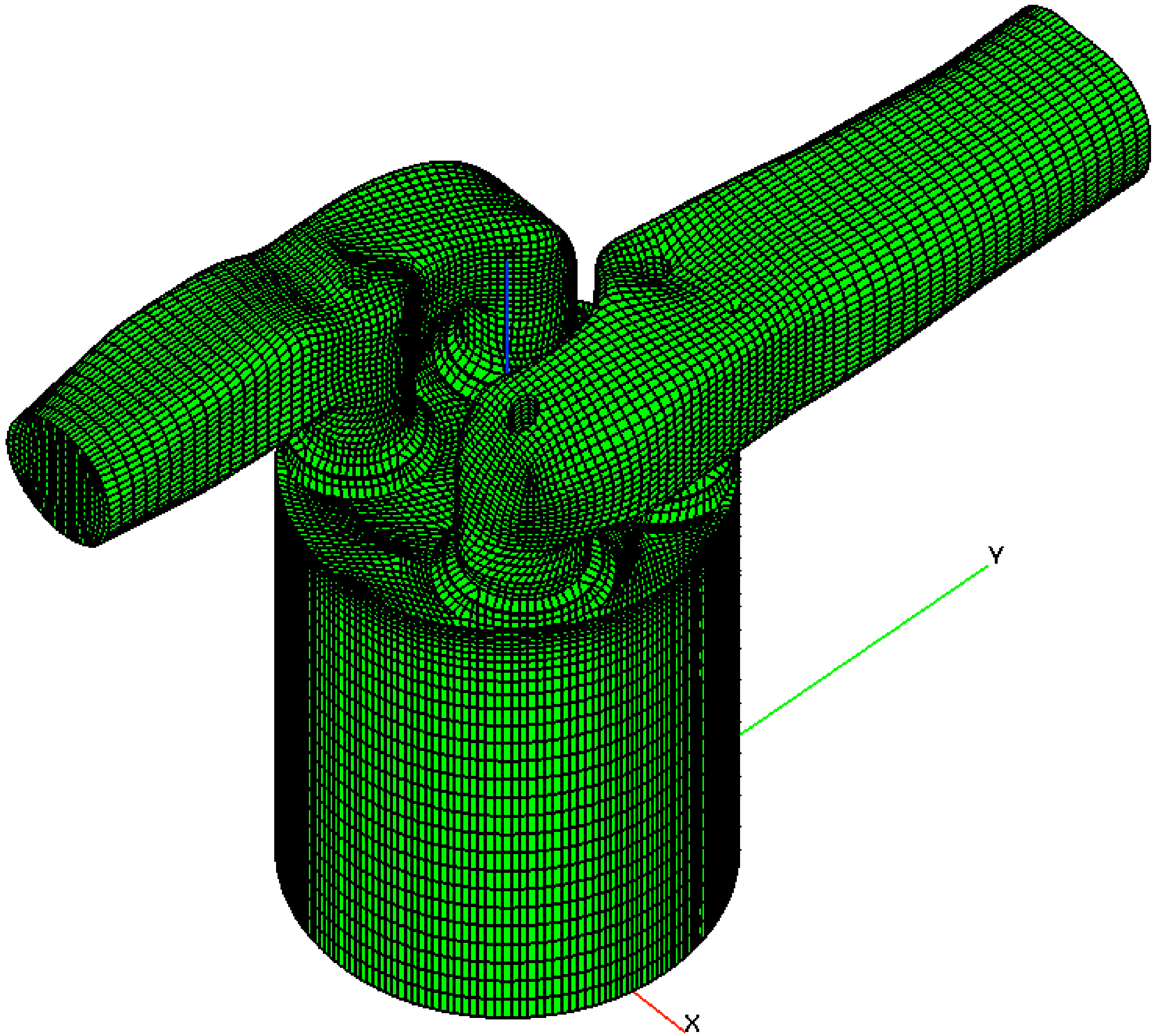


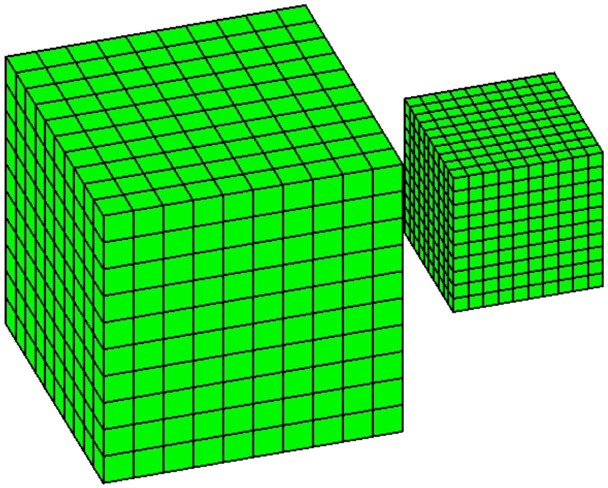
Mesh contributed by J.Y. Chen of U.C. Berkeley

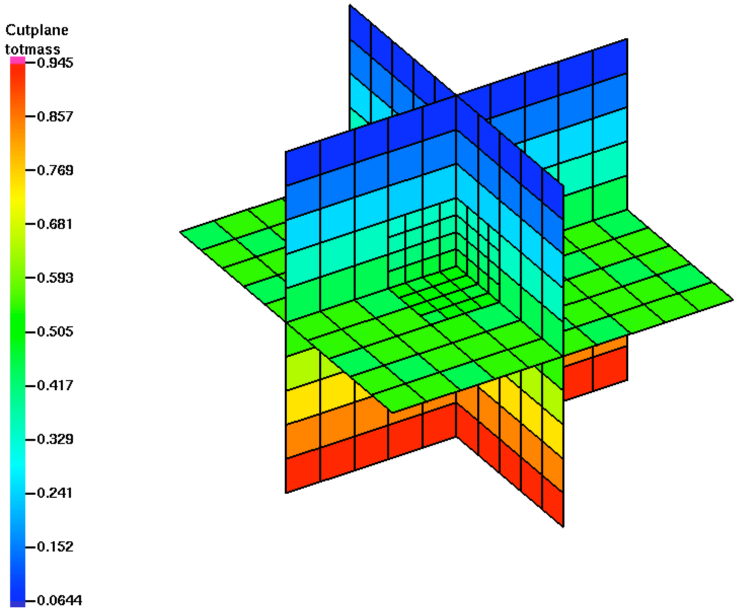
Reducing Spray Dependence

- 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.




Cutplane
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0.769
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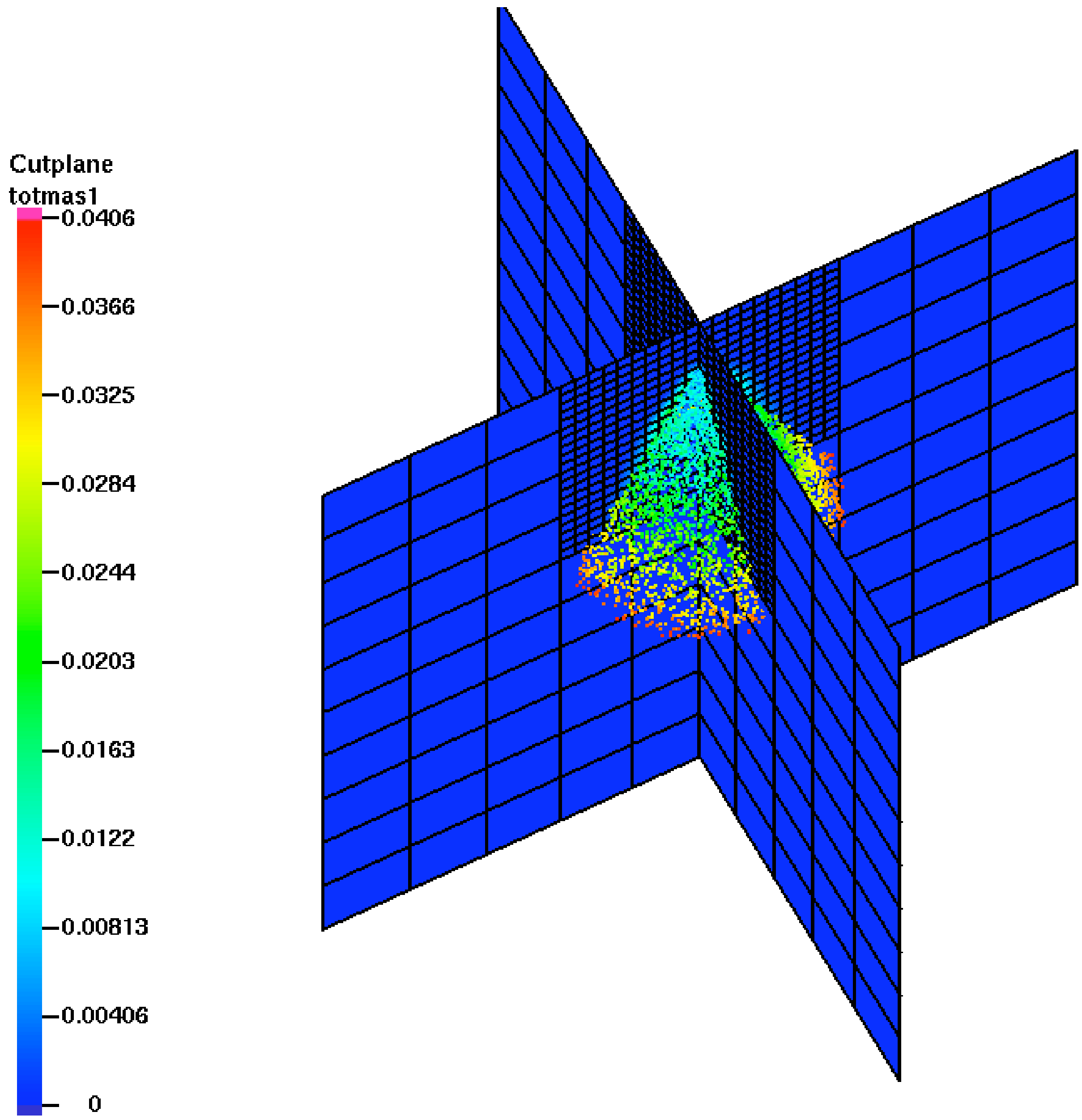
0.329
0.241
0.152
0.0644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0.0366
0.0325
0.0284
0.0244
0.0203
0.0163
0.0122
0.00813
0.00406
0

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.
  - Testing of realistic engine geometries in parallel in KIVA-4.
- 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.

Publications

- Xue,Q., S.C. Kong, D.J. Torres, Z. Xu and J. Yi, DISI Spray Modeling using Local Mesh Refinement, SAE 2008-01-0967.
- Fife, M., P. Miles, M. Bergin, R. Reitz and D.J. Torres, The Impact of a Non-Linear Turbulent Stress Relationship on Simulations of Flow and Combustion in an HSDI Diesel Engine, SAE 2008-01-1363.
- Torres,D.J., Colocated KIVA-4, International Multidimensional Engine Modeling User's Group Meeting at the SAE Congress (2007).
- Torres, D.J. and Mario Trujillo, KIVA-4: An Unstructured ALE code for compressible gas flow with sprays, Journal of Computational Physics, 219 (2006) 943-975.
- Torres,D.J., Parallel KIVA-4, International Multidimensional Engine Modeling User's Group Meeting at the SAE Congress (2006).
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- Torres, D.J., KIVA-4: Validation, Rezoning and Remapping, 15th International Multidimensional Engine Modeling User's Group Meeting at the SAE Congress (2005).
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- Trujillo, M.F., Torres, D.J. and P.J. O'Rourke, High-pressure multicomponent liquid sprays: departure from ideal behavior, International Journal of Engine Research, 5 (2004) 229-246.
- Torres, D.J., P.J. O'Rourke and A.A. Amsden, A discrete multicomponent fuel model, Atomization and Sprays, 13 (2003) 131-172.
- Torres, D.J., P.J. O'Rourke and A.A. Amsden, Efficient multicomponent fuel algorithm, Combustion Theory and Modelling, 7 (2003) 67-86.

Plans for Next Fiscal Year

- Continue LES turbulence model simulations in KIVA-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).

Summary

- 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.