Modeling of high efficiency clean combustion engines

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Overview

Timeline
- Start date: October 2005
- End date: September 2012
- Percent complete: 60%

Budget
- Total project funding
  - DOE share: $4M
- FY09 Funding: $1M
- FY08 Funding: $1M

Barriers
- Inadequate understanding of the fundamentals of LTC
- Inadequate understanding of the fundamentals of mixed mode operation

Partners
- Sandia Livermore
- Oak Ridge
- Los Alamos
- International
- UC Berkeley
- University of Wisconsin
- University of Michigan
- Chalmers University
- FACE working group
- SAE
Objective: Enhance understanding of clean and efficient engine operation through detailed numerical modeling

Chemical kinetics

Fluid mechanics
Milestones: We have developed and experimentally validated detailed engine modeling tools

- **Demonstrated accurate prediction of partially stratified combustion** (January 2009)
- **Developed improved surrogate chemical kinetic model for gasoline** (January 2009)
- **Analyzed SI-HCCI transition in ORNL experiment** (March 2009)
- **Calculated PCCI combustion with an artificial neural network-based chemical kinetic model** (March 2009)
Approach: collaborate with industry, academia and national labs in the development of analysis tools leading to clean, efficient engines

- Improved Chemkin multizone numerics
- Analysis of HCCI-SI transition
- Gasoline surrogate mechanism
- PCCI modeling
Accomplishments: The Newton-Raphson method efficiently solves nonlinear equations

\[ x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \]
When solving a system of differential equations,

\[
\frac{\dot{y}_i - y_i}{\Delta t} = f_i(\hat{y}_1, \ldots, \hat{y}_N) \quad \text{where } y_i = y_i(t) \text{ and } \hat{y}_i = y_i(t + \Delta t)
\]

the Jacobian matrix \( J = \frac{\partial f_i}{\partial y_j} \) plays the role of the derivative.

\[
(I - \Delta t \frac{\partial f_i}{\partial y_j}) (\hat{y}_j^{k+1} - \hat{y}_j^k) = -\hat{y}_i^k + y_i + \Delta t f_i(\hat{y}_1^k, \ldots, \hat{y}_N^k)
\]

\[
\frac{\partial f_i}{\partial y_j} = \begin{pmatrix}
\frac{\partial f_1}{\partial y_1} & \cdots & \frac{\partial f_1}{\partial y_N} \\
\vdots & \ddots & \vdots \\
\frac{\partial f_N}{\partial y_1} & \cdots & \frac{\partial f_N}{\partial y_N}
\end{pmatrix}
\]
Processing the Jacobian is the most computationally expensive part of CHEMKIN-Multizone

- 94% of the total computational cost is spent generating the Jacobian and solving the associated linear system.

![Computational breakdown of the CHEMKIN-Multizone model](image)

- 32M calls to the CHEMKIN species production rate
- 4400 Gaussian eliminations for 1300 x 1300 system
Chemkin multizone produces a block-diagonal Jacobian. Can we take advantage for reduced computational time?
New procedure: use LLNL’s ODE integrator with an iterative matrix solver (DLSODPK)

- Use LLNL’s iterative solver DLSODPK along with a preconditioner matrix $P$
  $$P^{-1}Ax = P^{-1}b$$
- Here $P$ is the Jacobian of a simplified CHEMKIN-multizone model that yields a block diagonal matrix (neglecting interaction between zones)
The new DLSODPK scheme accelerates computations enabling detailed multizone kinetics on desktop PCs.

Computational breakdown of the CHEMKIN - Multizone model:

- 17x fewer calls to CHEMKIN species production rate
- Total Gaussian elimination cost is +400x smaller

60x speedup for 20 zones; 6 minutes (6 hours) with 63 species
250x speedup for 40 zones; 24 minutes (100 hours) 63 species
We are analyzing ORNL results for stability and emissions during SI-HCCI transition due to increased residual gas fraction.
1-dimensional chemical kinetic model accurately matches pressure traces for motored, SI and HCCI cases

- Spark-ignited
- HCCI (EGR=74.7%)
ORNL Test data for SI to HCCI transition: heat release patterns vary with residual gas fraction

Spark-ignited (EGR~10%) Increasing EGR

HCCI (EGR~60%)
LLNL Simulation results for SI to HCCI transition: heat release patterns vary with residual gas fraction

Spark-ignited (EGR~10%)  Increasing EGR

HCCI (EGR~60%)
HCCI is more than a promising engine operating regime. HCCI is also an excellent platform for developing & testing high fidelity chemical kinetic models.

- n-heptane
- methylcyclohexane
- toluene
- iso-octane
- 1-pentene

Detailed kinetics of gasoline surrogates

High fidelity engine models
Gasoline surrogate model accurately predicts ignition time as a function of equivalence ratio.
But it does not properly replicate ignition time as a function of intake pressure
Analysis of pressure sensitivity of low temperature reaction steps may offer guidance toward improving quality of agreement.
Increasing the reactivity of the radical recombination reaction $R + O_2 \rightarrow RO_2$ matches experimental results up to ~1.7 bar intake.
We obtain improved agreement by reducing activation energy of chain branching reactions as a function of pressure.
We are analyzing three consecutive cycles of the Sandia automotive PCCI engine (Steeper)

Sandia Automotive HCCI Engine
operated by Dick Steeper
PHI = 0.293
1200 RPM

Visualized species and what is represented:
CO: incomplete combustion
Hi concentration
Low concentration

CA = -375

CFD by:
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The Sandia engine runs in PCCI mode with dual injection: one injection during NVO and a main injection.

NVO = 150 crank deg.  
Fired case

Injections:
- NVO
- Main

150 ca deg.
KIVA3V-MZ-MPI shows promise for accurately predicting direct injected PCCI

NVO150 Fired case

- measured
- calc, cycle2

Crank angle, deg. atdc

Pressure, MPa

exp. 80227ai
Future work: we are preparing our codes for public release

Chemkin multizone
(1-D flame propagation & autoignition)

KIVA-multizone
(HCCI, PCCI)

KIVA-sequential multizone
(HCCI)

KIVA-artificial neural network
(HCCI, PCCI)
Future work: extend applicability and computational efficiency of analysis tools

HCCI-based chemical kinetic mechanism testing and tuning

Full PCCI validation
KIVA-MZ, KIVA-ANN

Enable 3-D fluid mechanics and detailed kinetics in today’s desktop PCs
Summary: we are enhancing our analysis capabilities and improving computational performance

- 60x-250x Improved numerics
- HCCI-SI transition modeling
- Gasoline surrogate
- Partially stratified combustion

Graphs and data visualizations illustrating the improvements in computation and simulations.