Application of CFD Simulation to Low-Temperature Combustion of Biofuels

2006 Presidential State of the Union Address: announced goal of reducing imports of foreign oil… and increase national competitiveness by use and development of advance energy technologies.

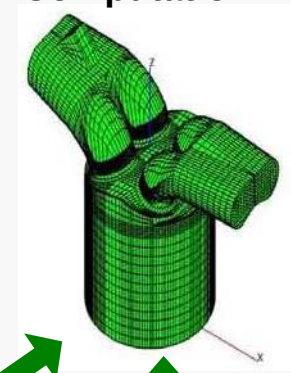
Joanna McFarlane

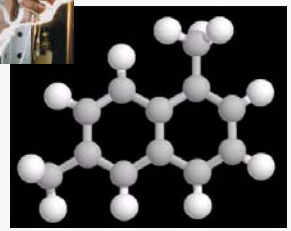
CFD Workshop

ORNL December 15 2006

ORNL LDRD Project on the Simulation of Combustion of Alternative (Non-Petroleum) Fuels:

Computation





Fuel Chemistry

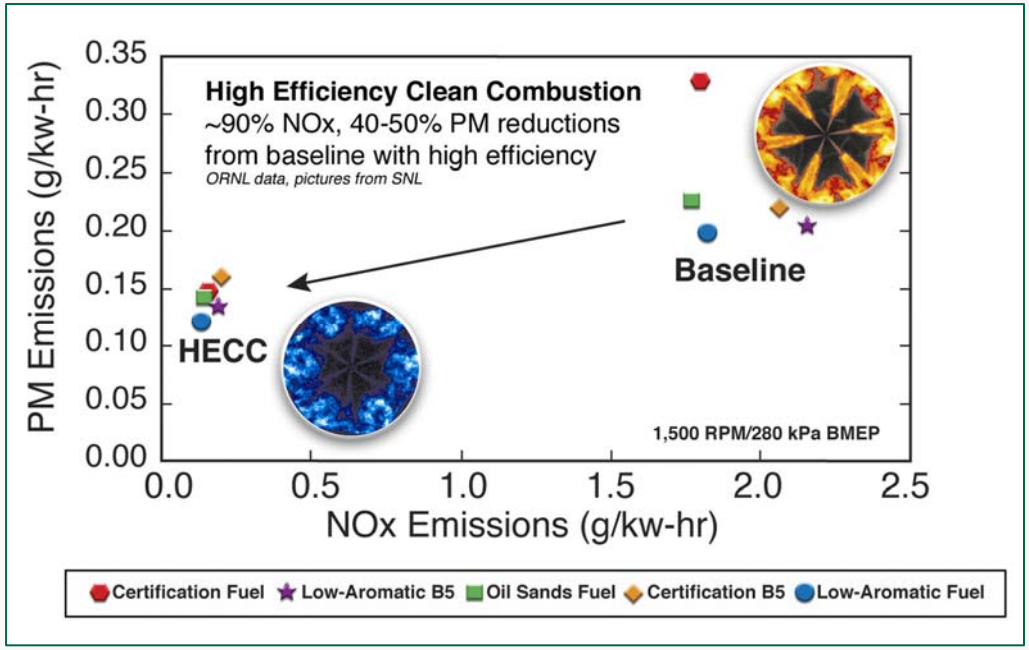
Experimental

- **Develop predictive tool to evaluate high-efficiency combustion of alternative fuels**

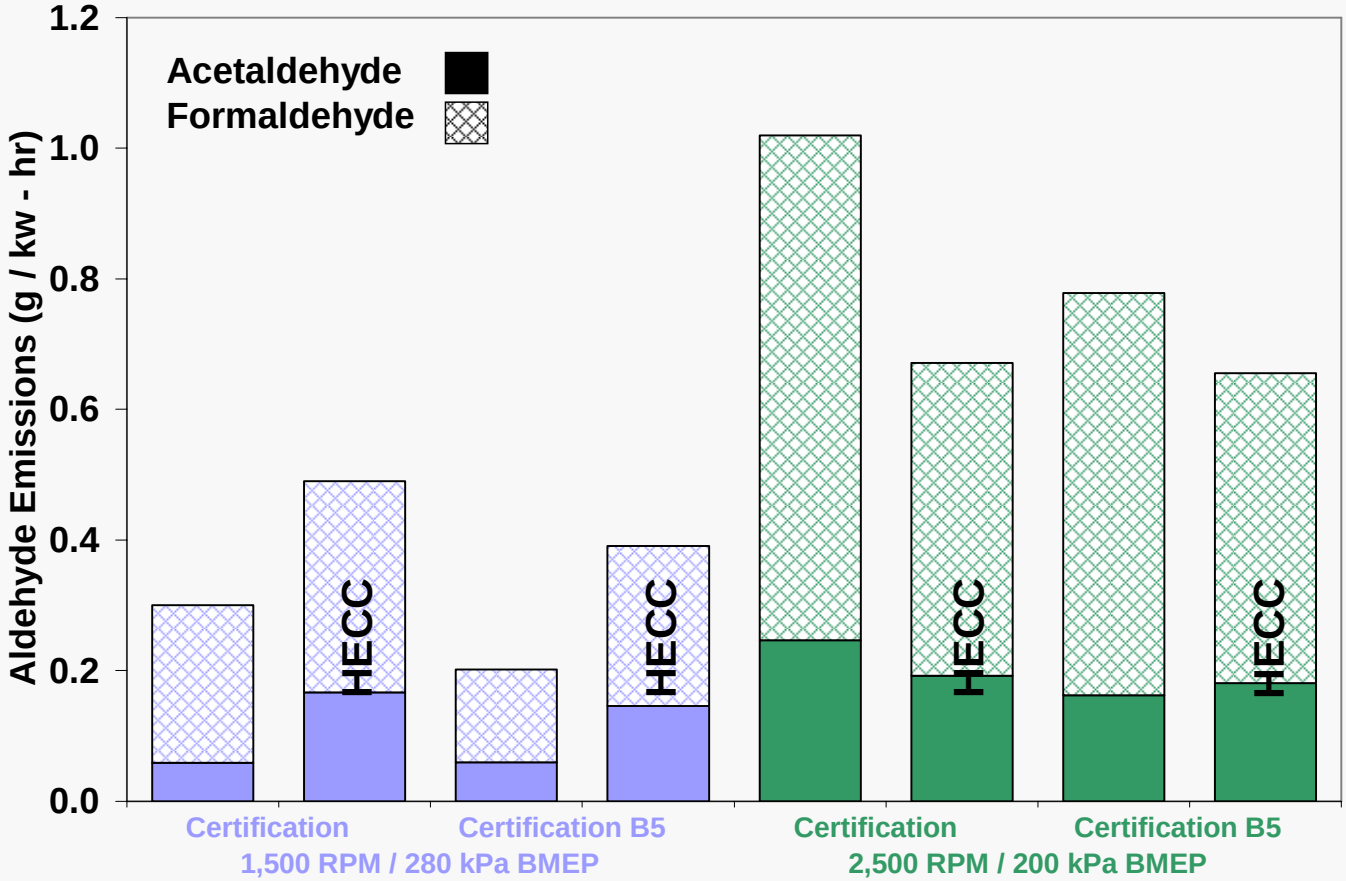
- **Combine capabilities in fuel chemistry and engineering computations with established strength in IC engine experimentation to create a unique R&D program**

Advanced combustion modes will be used on some level in all future transportation engines

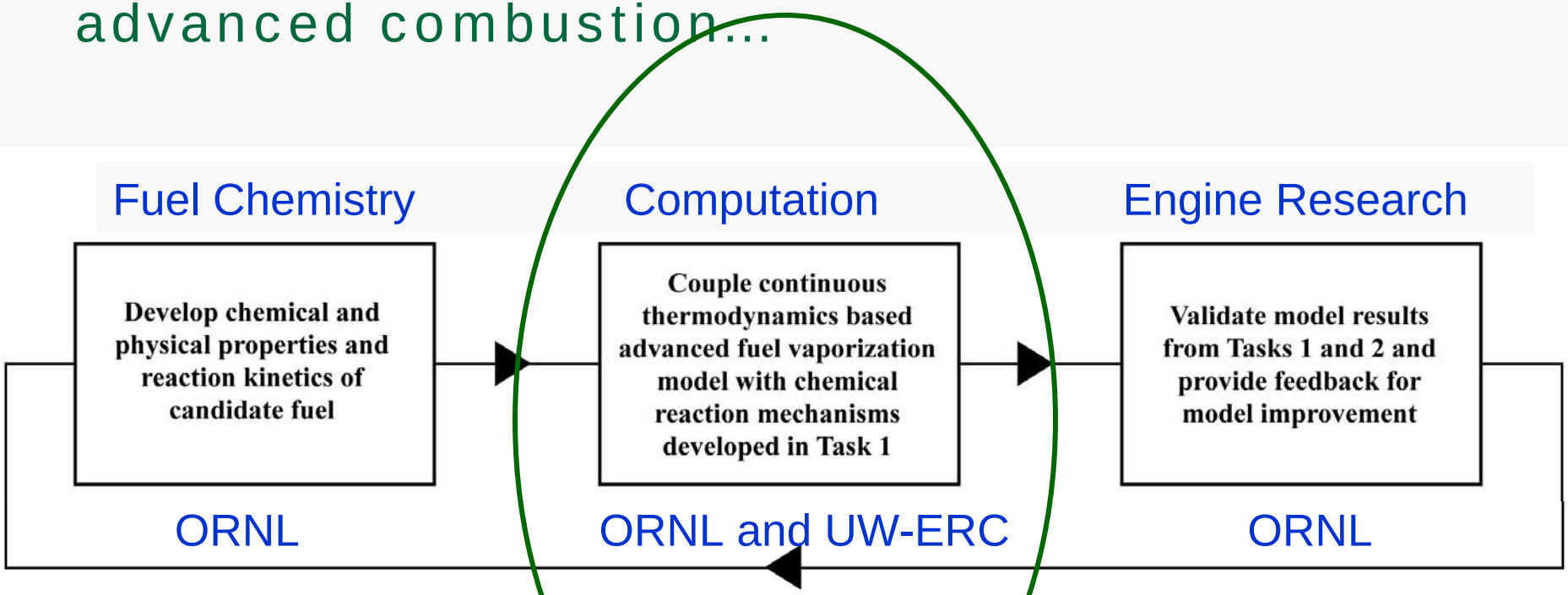
- **Advanced combustion characterized by low temperature combustion (LTC) processes: low emissions and improved efficiency.**
- **Typically less stable than conventional forms of combustion (i.e., sensitive to air-fuel charge conditions including fuel properties).**
- **Several forms of LTC exist including Homogeneous Charge Compression Ignition (HCCI), Premixed Charge Compression Ignition (PCCI), etc.**
- **Modes are commonly referred to as High Efficiency Clean Combustion (HECC) in the literature.**



Adding biodiesel changes emissions of HC, NOx, and aldehydes.



Project to analyze and simulate effect of fuel on advanced combustion...



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LANL KIVA Code Evolution

- Version 2 (1989)
  - In-cylinder, 3-D, multi-species, chemically reactive, turbulent, "confined", gas flow
  - Single-specie, multi-component discrete fuel spray particle
  - Single-block structured mesh
  - Fuel library
- Version 3 (1993)
  - Block-structured mesh
  - Cylinder side inlet/outlet ports
- Version 3V (1997), Release 2 (1999)
  - Vertical and canted valves
  - Particle-based liquid wall film model
  - Soot model
- Version 4 (available on request to the developer)
  - Unstructured mesh
  - Multiple fuel species evaporation

U. Wisconsin ERC has developed submodels for spray droplet formation, soot formation

Increase data requirements

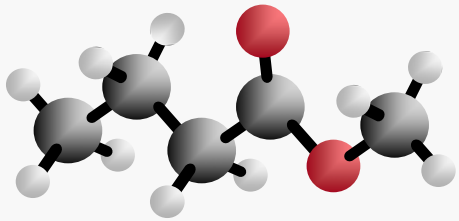
Need Data
For Fuels:
Physical properties
Combustion kinetics
For Engine: Mesh

Modeling Components

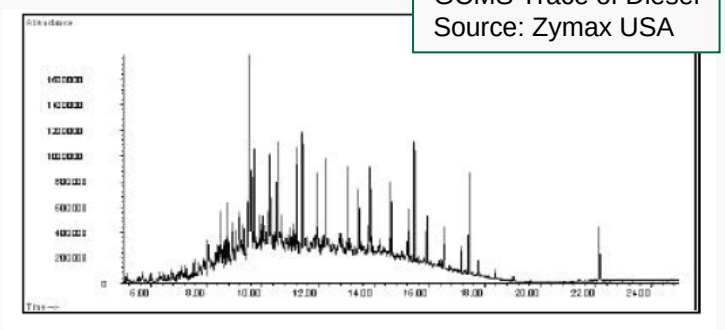
1. Multi-species Gas Flow
2. Chemical Reactions
3. Spray Droplets
4. In-Cylinder
5. Sub-models

coupled

Chemical studies to develop a realistic reaction set for alternative fuels



- **Consider bio-derived mixtures (e.g., methyl esters, alcohols)**
- **Calculate fuel physical properties**
- **Define reaction mechanisms**
  - **Combustion of real multi-component fuels involves hundreds of species and thousands of reactions (n-heptane, methyl butanoate, NOx, long chain olefins – C16)**
- **Evaluate reaction kinetics for use in CFD**
  - **Develop reduced mechanism**
  - **Senkin for sensitivity analysis**
    - **ERC: nheptane, iso-octane, mb**
    - **Fit reaction coeff to data**
  - **XChemKin exploratory tool**
    - **Work with unreduced mechanism**
    - **PCA analysis**



GCMS Trace of Diesel
Source: Zymax USA

XChemKin Architecture

$$\partial_t(\rho u) + \mathrm{div}_x(\rho v u) = -p\,\mathrm{div}_x v + \tau : \nabla_x u - \mathrm{div}_x q + Q^F + Q^R$$

$$\partial_t \rho_m + \mathrm{div}_x(\rho_m v) = \mathrm{div}_x(\rho D\, \nabla_x(\rho_m \rho^{-1})) + \dot{\rho}^c_m + \dot{\rho}^R \delta_{m1}$$

Model
(CHEMKIN III)

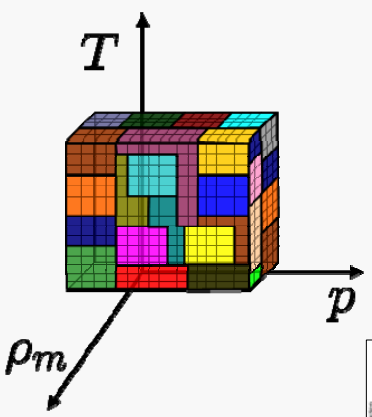
XChemKin

Mechanism

1540 reactions (n-heptane LLNL)

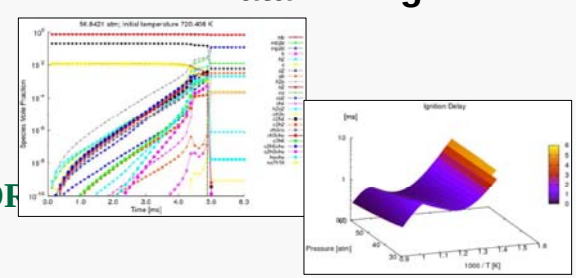
561 species

Phase Space Partitioning



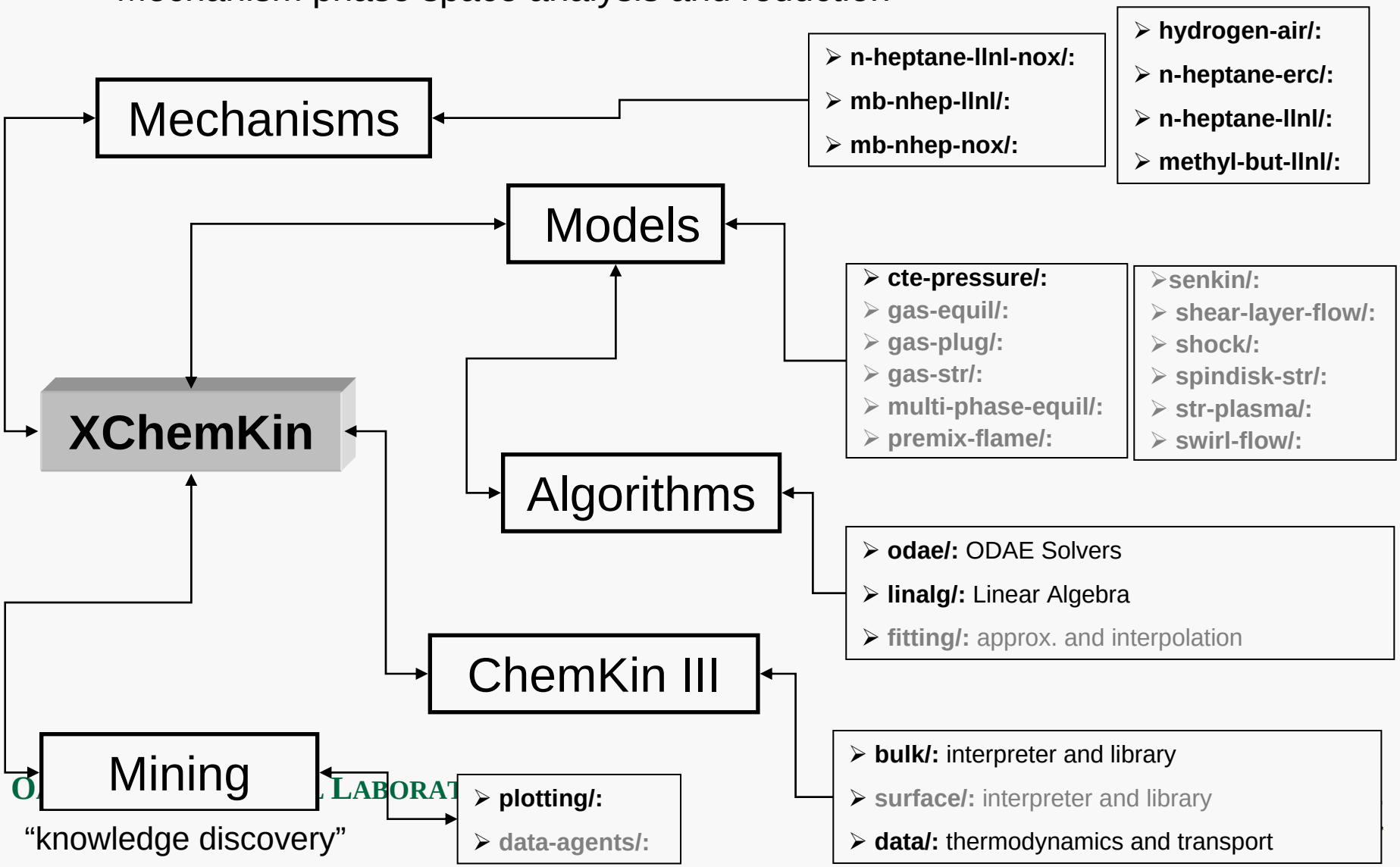
Parallel Computing

Data Mining



XChemKin Architecture

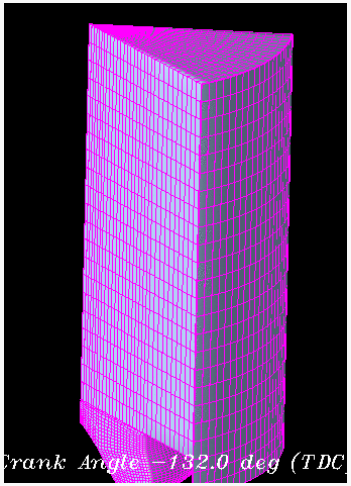
- Exploratory tool for chemical kinetics modeling
  - Mechanism phase space analysis and reduction



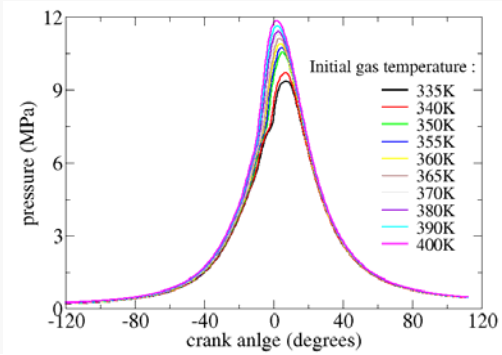
"knowledge discovery"

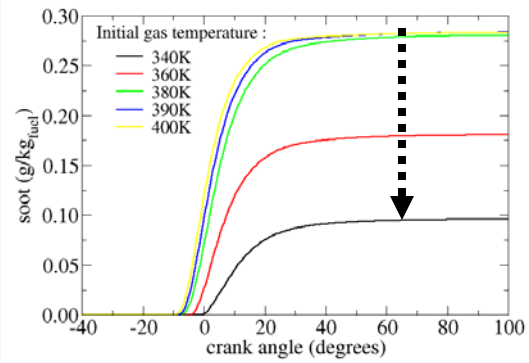
KIVA-3ERC in-cylinder combustion simulations for reference case

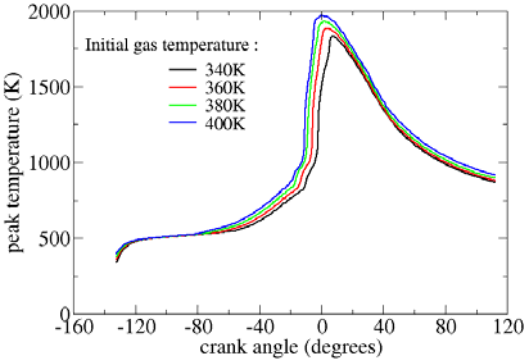
- **KIVA-3 U of Wisconsin ERC version running on ORNL cluster**
- **Simulation of diesel spray combustion on GM engine**
  - **ERC n-heptane reduced model (29 species, 54 reactions)**
- **Parametric studies on EGR**
- **Simulation of HCCI, PCCI**

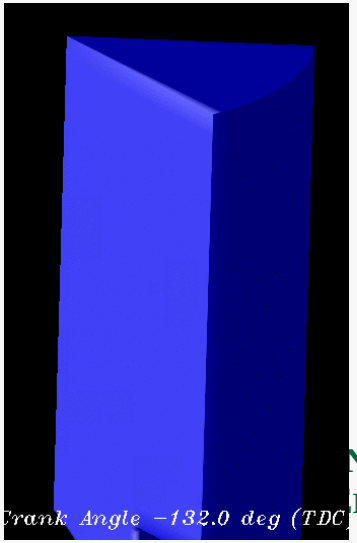


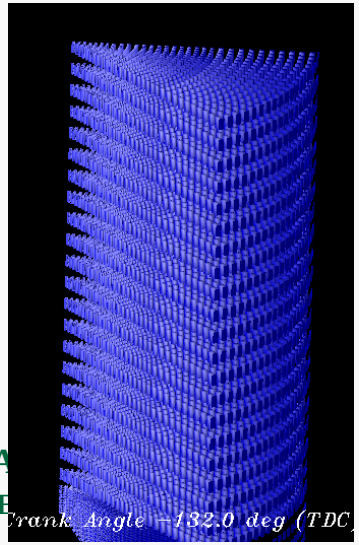
Youngchul Ra, U. Wisconsin ERC, Post –doc collaborator

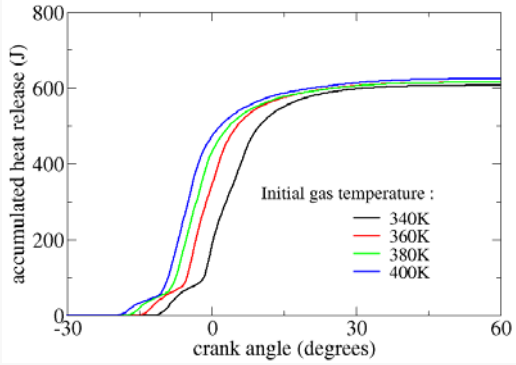


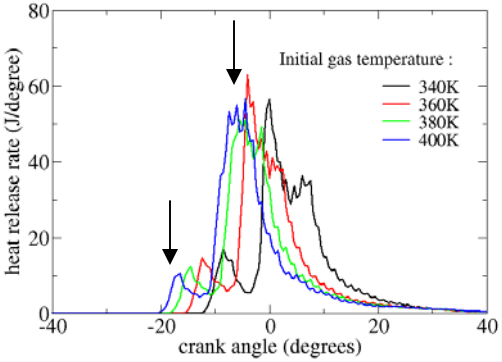












Pressure and Heat release rate profiles for PCCI in GM Engine

<u>Operating conditions</u>

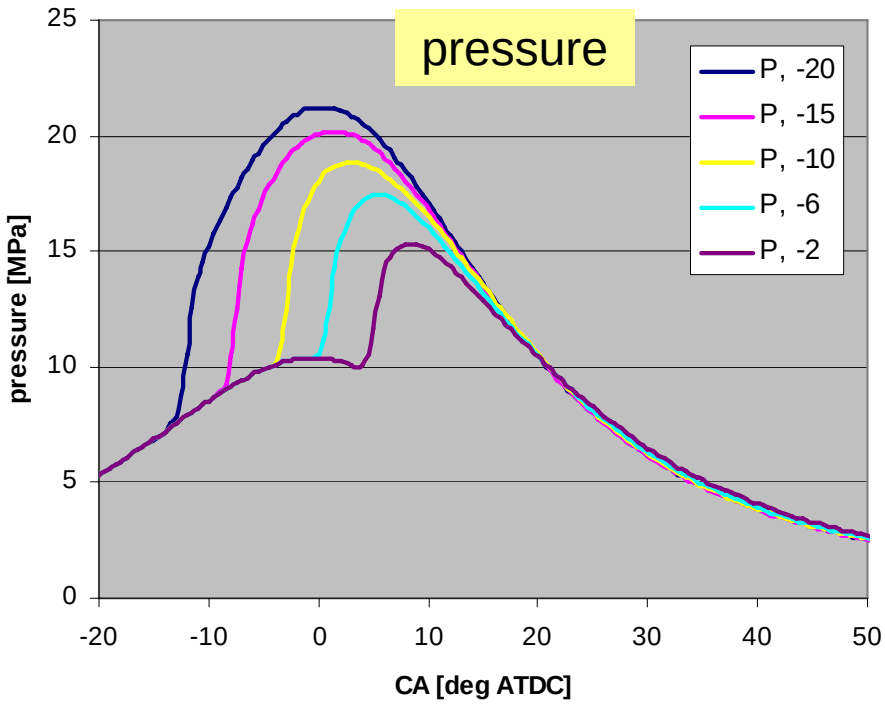
CR=19.2, EGR=40%, Equivalence ratio = 0.75

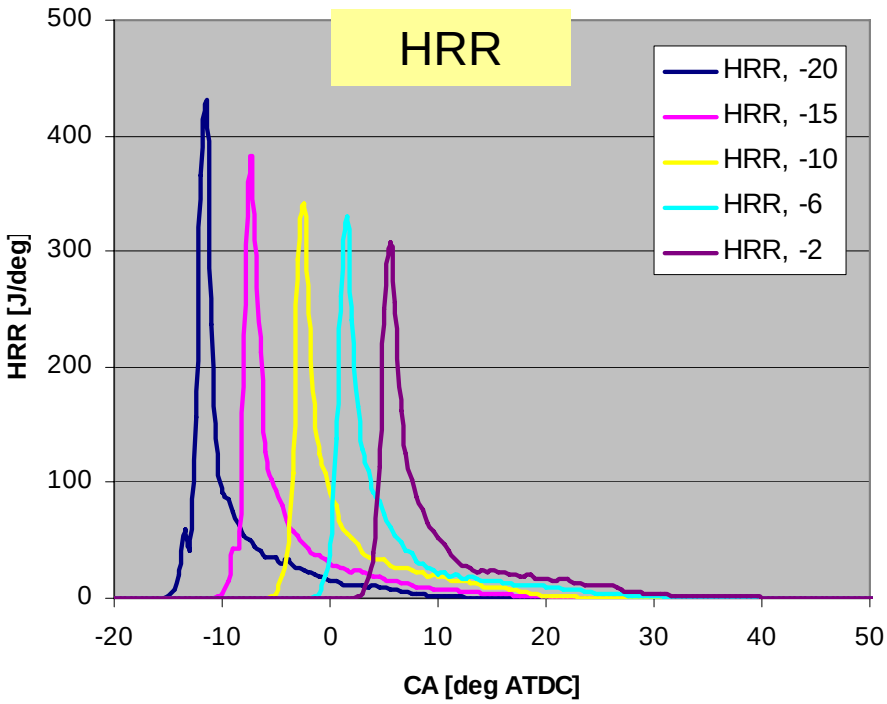
RPM=1500, Injection duration=4.04 deg CA

GM engine with 7-hole injector

Pivc=2.36 bar, Tivc=373.15 K

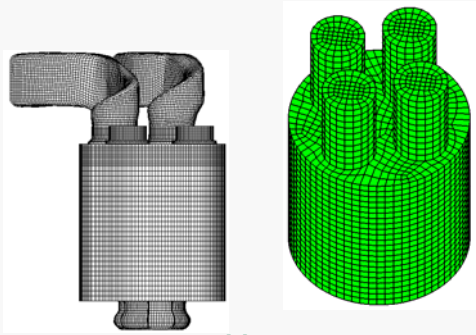
Injection timing variation: -20 ~ -2 deg ATDC



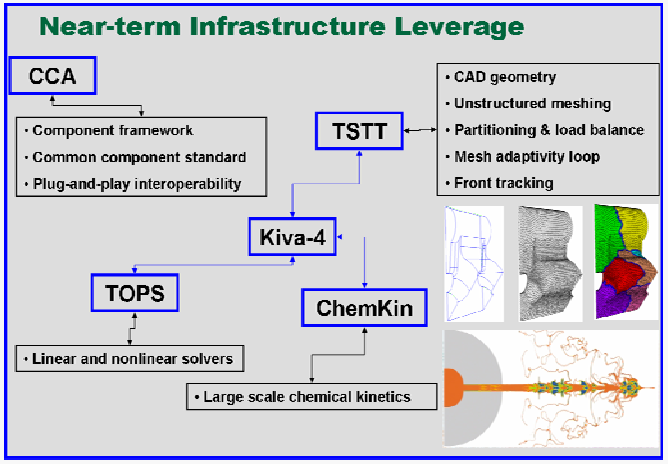


Participation in KIVA-4 development

- KIVA-4 is the successor of KIVA-3
  - High-performance computing
  - All-parallel, unstructured mesh
- Development supported by DOE EERE OFCVT (PI: David Torres at LANL)
- ORNL leveraging high-performance computational tools from the SciDAC program for geometry, meshing and parallelization
- ORNL/SUNY Stony Brook advanced spray modeling for KIVA-4
  - Profs. James Glimm and Xiaolin Li
  - Prof. Zhiliang Zhu
  - interface tracking for spray modeling

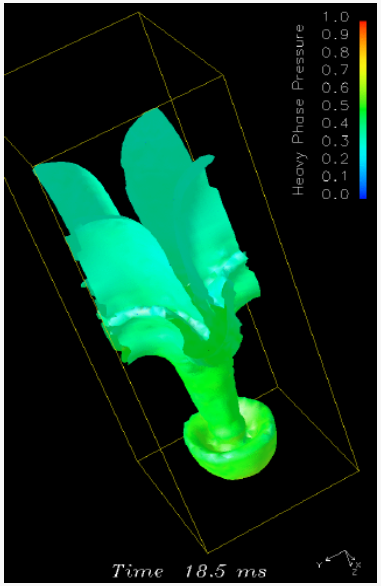


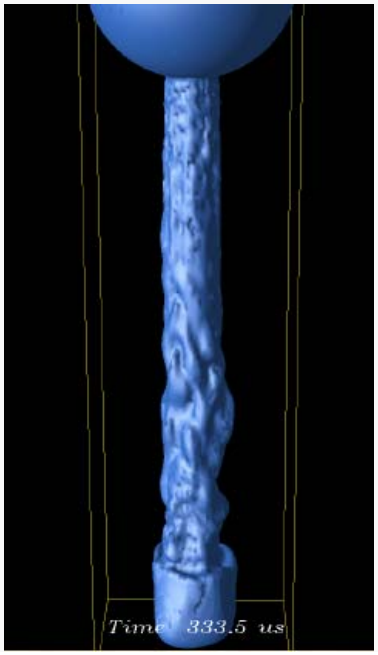
David Torres
Merit Review of Advanced Combustion, Emissions Control and Fuels Research
May 15-18, 2006

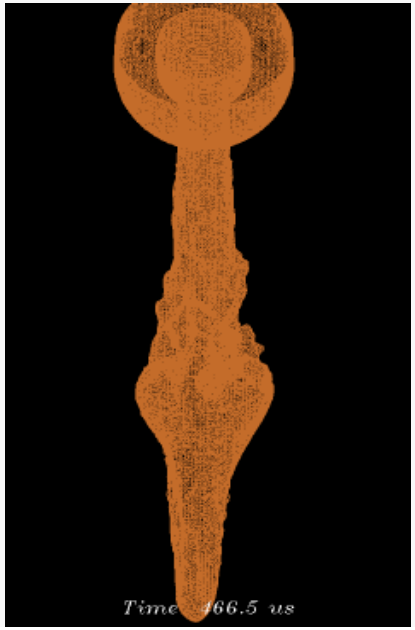


Spray Model Development

- **Engine Research Center Model used in KIVA 3**
  - **Parametric study on sensitivity of ERC spray model to fuel properties**
  - **Extend to multi-component fuel, including evaporation and droplet breakup**
- **KIVA 4**
  - **Interface tracking**
  - **Single droplet dynamics**
  - **Jet (variation in density ratio, surface tension)**
  - **Cavitation/voids in vicinity of nozzle**

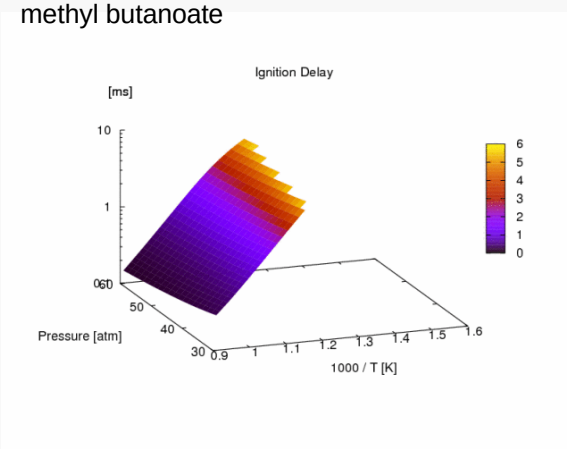




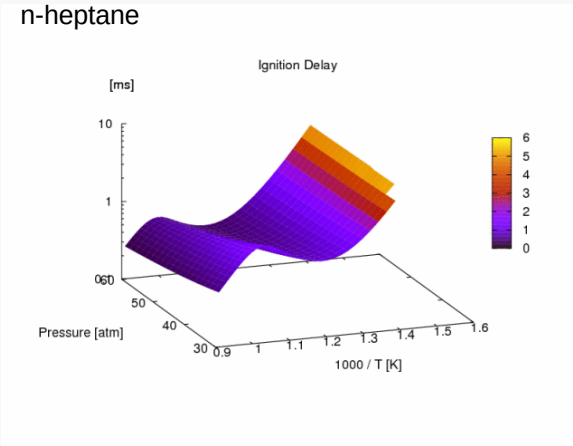


Engine Simulation and Validation to come....

methyl butanoate



n-heptane



- **Simulate ORNL engine experiments**
  - **Couple reduced mechanisms with engine mesh and fluid flow**
  - **Low temperature, HECC conditions, EGR 0-50%, alternative fuels**
  - **Track representative hydrocarbon species in exhaust, gas phase emissions, semi-volatiles, and the SOF**
- ***Integrate fuel chemistry, computational, and engine testing to develop a predictive tool to assess the compatibility of alternative fuel blends with advanced combustion modes***

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