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COMBUSTION RESEARCH FACILITY

Scientific and Engineering Challenges Impacting the Design of Advanced Internal Combustion Engines

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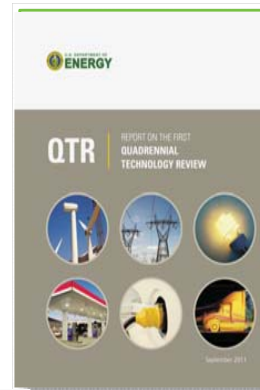
Unclassified, Unlimited Release

Acknowledgements: Gurpreet Singh, DOE EERE-OVT
General Motors Corporation

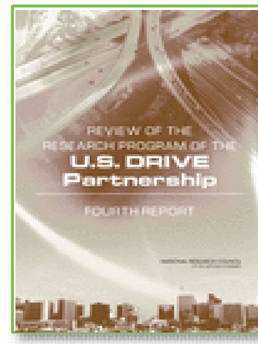
Part I:
US Department of Energy (DOE) Office of Vehicle Technologies

View of the Future, Program Goals & Overview

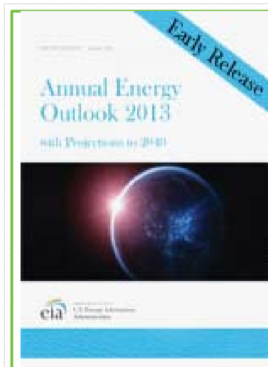
Internal Combustion Engines (ICEs) will dominate the vehicle fleet for several more decades



"The performance, low cost, and fuel flexibility of ICEs makes it likely that they will continue to dominate the vehicle fleet for at least the next several decades. ICE improvements can also be applied to both hybrid electric vehicles (HEVs) and vehicles that use alternative hydrocarbon fuels." [1]



"…ICEs … are going to be the dominant automotive technology for decades, whether in conventional vehicles, hybrid vehicles, PHEVs, biofueled or natural gas vehicles. [2]



Even by 2035, ***over 99% of vehicles sold will have ICEs*** [3]

1. Quadrennial Technology Review, DOE 2011
2. Review of the Research Program of the U.S. DRIVE Partnership: 4th Report, NRC 2013
3. Annual Energy Outlook 2013, Early Release, DOE 2012.

"ICEs are cost-effective, reliable, durable, and exhibit fuel flexibility"

DOE Advanced Engine Combustion Program

Strategic Goal: Reduce petroleum consumption by removing technical barriers to mass commercialization of high-efficiency, emissions-compliant ICEs

Advanced Combustion Engine R&D
$56.7M (FY13)

Thrust areas:

- **Advanced Combustion R&D** / **Emission Control R&D** — **$48.2M**
- **Solid State Energy Conversion** — **$8.5M**

Performance Targets:

	Light-Duty		Heavy-Duty	
	2015	2020	2015	2020
Engine brake thermal efficiency			50%	55%
Fuel economy improvement	25 – 40%	35 – 50%	20%	30%
NOx & PM emissions	Tier 2, Bin2	Tier 2, Bin2	EPA Standards	EPA Standards

Advanced Combustion Technical Barriers

- **Engine development inhibited by:**
  - Inadequate understanding of the fundamentals of fuel injection, fuel-air mixing, thermodynamic combustion losses, and in-cylinder combustion/ emission formation processes

    "For the operating points we used smoke has decreased by 11-27%, NOx has decreased by 2-11%, while efficiency is maintained or improved. Not a single operating point showed worse results than the baseline...

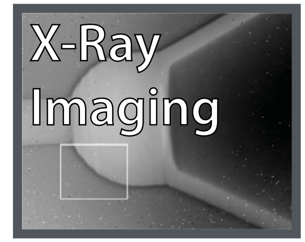
    ...The bottom line is that the mental image of the in-bowl processes you describe can really guide a bowl designer towards a better design"
  - Inadequate capability to accurately simulate these processes
- **Lack of Effective Controls**

  Injection and ignition timing, rate of heat release, transients, cold-start
- **Durability**

  Materials, lubricants, peak pressures
- **Cost**
- **Market/consumer acceptance**

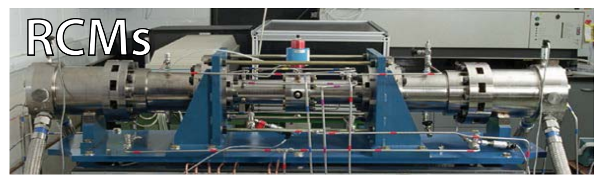
Advanced Combustion
Examples of supported projects: Experiments

Single-cylinder optical engines

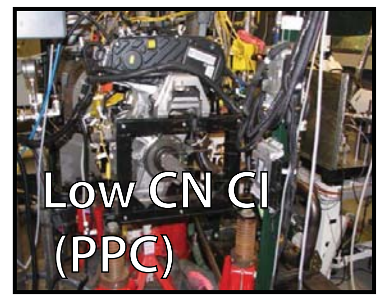


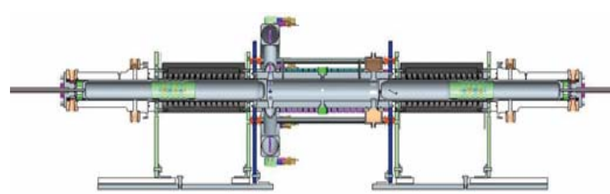
Fuel Inj. & Sprays

See www.sandia.gov/ecn/



Multi. & Single-Cyl. Test Engines / Benches

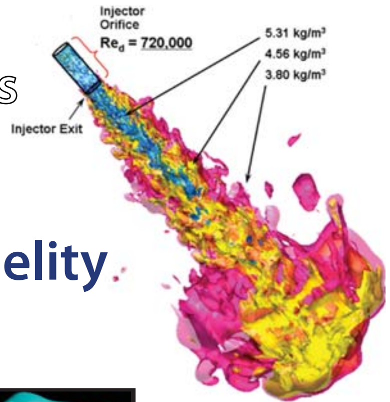




Free Piston / Linear. Alt.

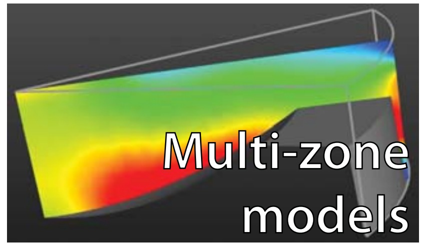
Advanced Combustion
Examples of supported projects: Simulation

Sprays



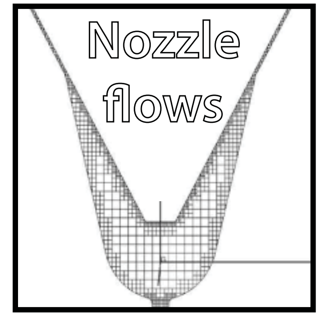
High Fidelity LES

Engine studies

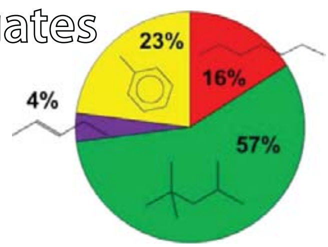


Engineering LES & RANS

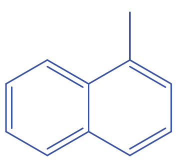
KIVA4-mpi
- *Parallel*
- *Finite element*
- *Unstructured mesh*



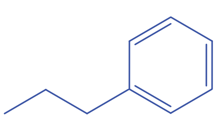
Fuel surrogates



Chemical Kinetics

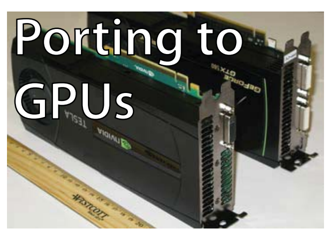


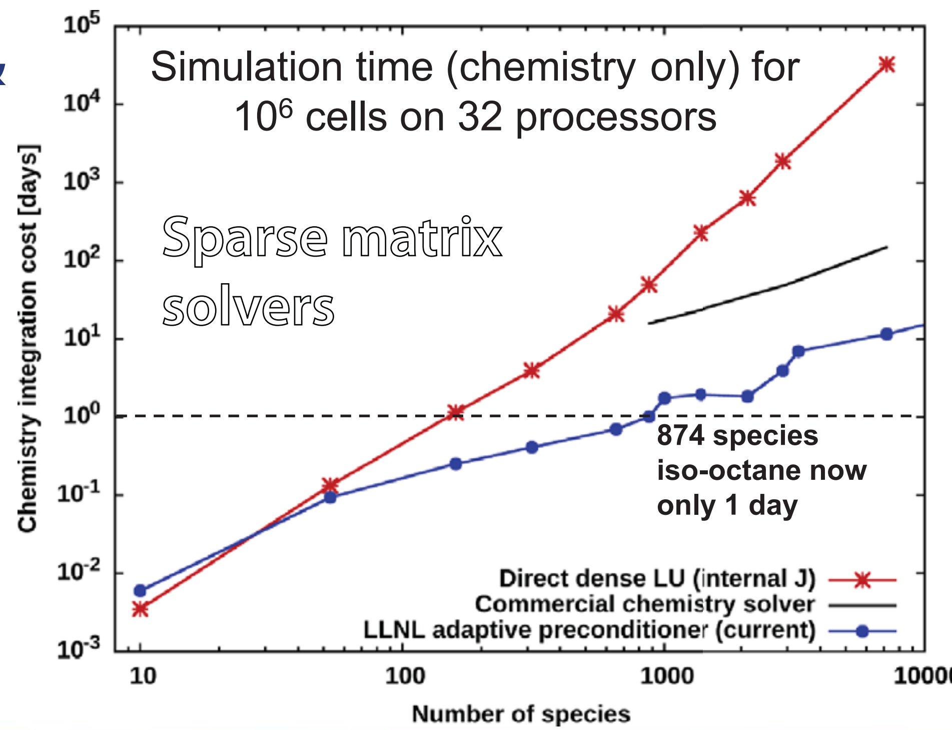
Mechanisms



Algorithms & Numerics

Tesla K20
2496 Cores
@$2,895.99





Emission Control Technical Barriers

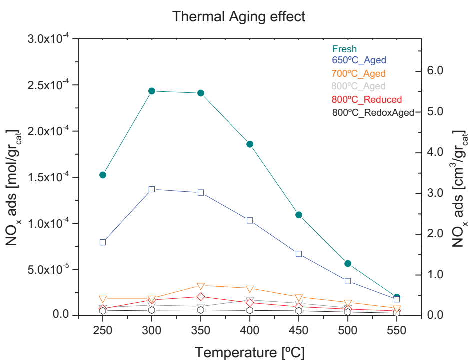
- Deficiencies in fundamental understanding and modeling capabilities
- Need high effectiveness over broader temperature range (cold start)
- Inadequate sensors for process control or diagnostics
- Inadequate methods for rapid-aging
- Cost/Packaging constraints on the vehicle
- NOx after-treatment
  - Degradation from sulfur (even at 15 ppm) and thermal processes
  - NOx adsorbers: fuel penalty, conv. efficiency vs. temperature, Pt content, sulfur poisoning
  - Selective Catalytic Reduction (SCR): catalyst deactivation, incomplete reaction products
  - Ineff. engine mgmt. for regeneration and desulfation (LNT); poor reductant utilization (SCR)
- PM after-treatment
  - Regeneration strategy, DI gasoline, particle number and size regulation
- HC/CO
  - Hydrocarbon SCR: conversion efficiency temperature window, early development stage
  - Oxidation catalysts: high temperature durability, HC & CO oxidation efficiency

Emission Control Projects

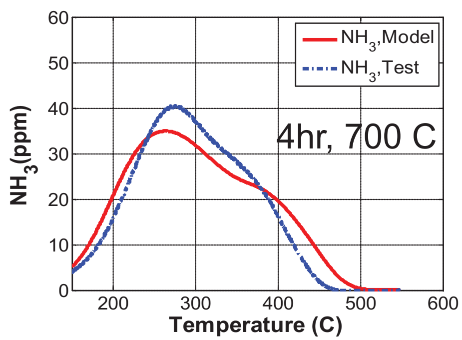
Technical Focal areas:

- Systems with 90% conversion of all emissions below 200C
- Mechanisms of catalyst deactivation
- PM from DI gasoline due to new regulations, different size/morphology vs. diesel

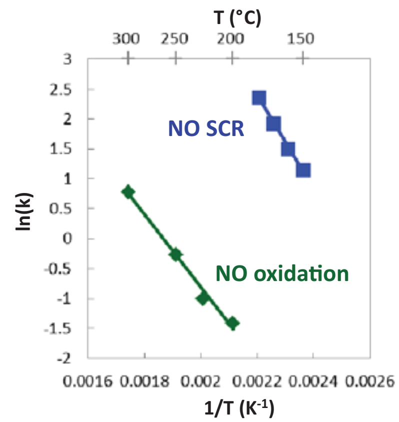
Example projects:



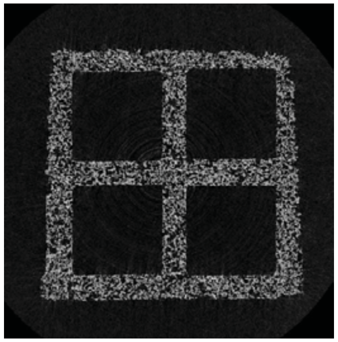
LNT testing



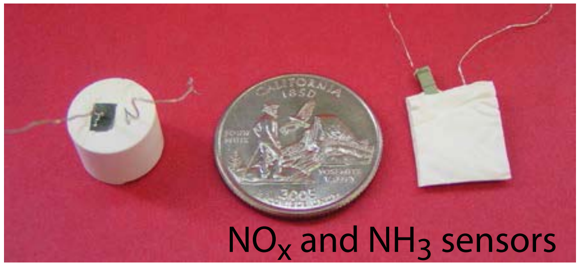
NH_3 storage modeling



SCR Cu zeolite kinetics



High resolution imaging of PM filter loading



NO_x and NH_3 sensors

Collaborative health effects studies with Health Effects Institute (HEI), Southwest Research Institute, Lovelace Respiratory Research Institute, and Coordinating Research Council (CRC)

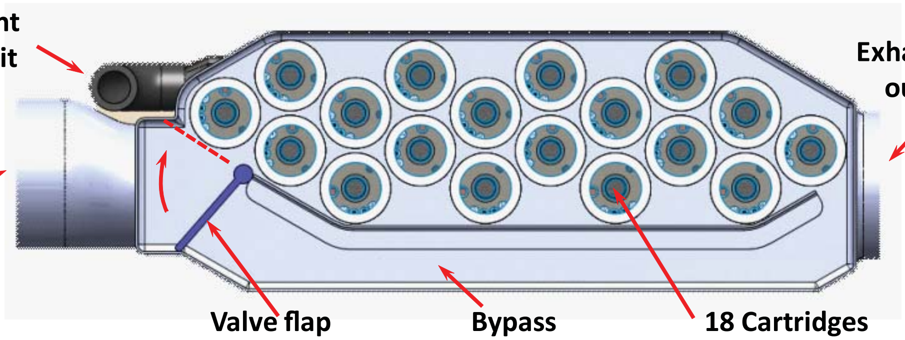
For more information: www.cleers.org

Crosscut Lean Exhaust Emissions Reduction Simulation

Solid State Energy Conversion Barriers & Projects

Barriers/Challenges:

- Cost
- Scale-up to a practical device
- Device/System Packaging
- Inadequate methods for rapid-aging
- Component/System durability



Focus on materials & demonstration projects

- Competitively selected cost-shared 2nd Gen TEG projects:
  - GenTherm
  - General Motors
  - GMZ Energy

Develop commercially viable advanced TEGs, improved technology for manufacturing TE devices, and assess feasibility and cost reduction for production volumes of 100,000 units

- NSF and DOE/VTP MOU on automotive thermoelectric materials development

National Science Foundation
Directorate for Engineering
Division of Chemical, Bioengineering, Environmental and Transport Systems

Projects coordinated with:

USDRIVE
DRIVING RESEARCH AND INNOVATION FOR VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

21st CENTURY TRUCK PARTNERSHIP

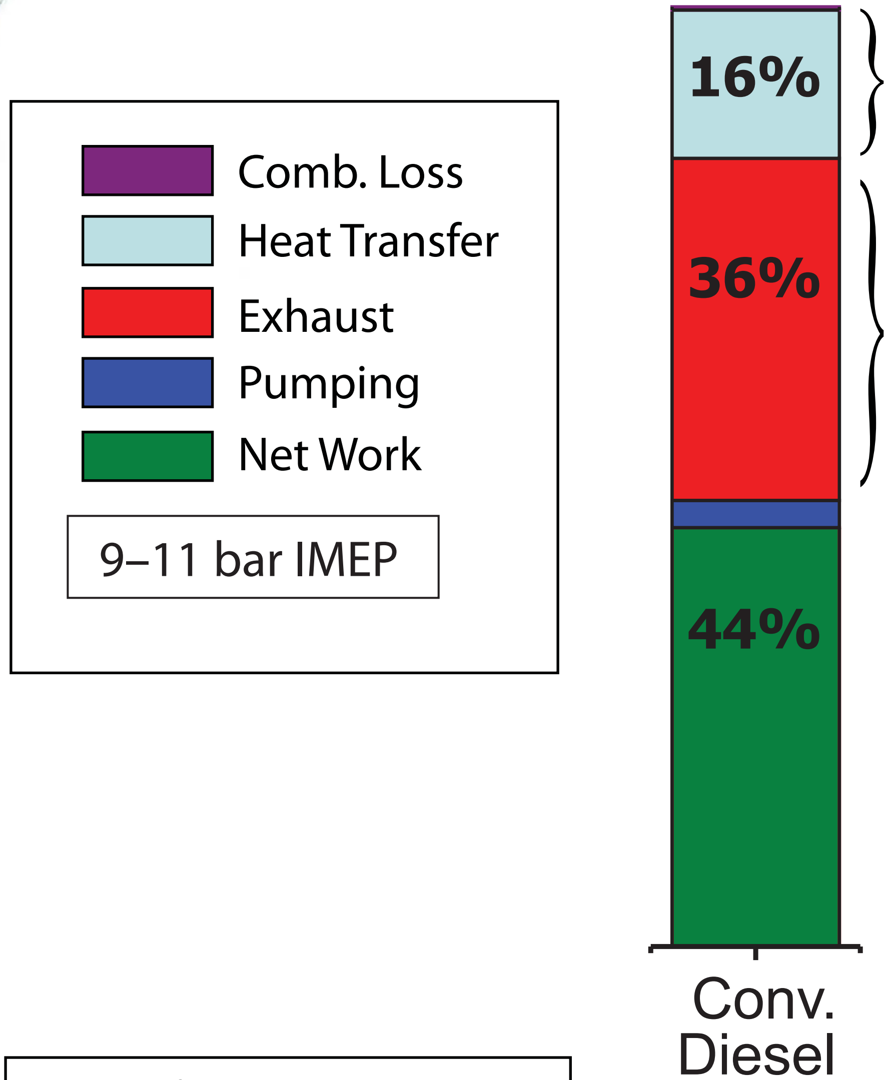
Part II:
Scientific & Engineering Challenges

Over the next 20 years, IC engines will remain dominant and will not change dramatically in architecture

Vehicle efficiency can be impacted by:

- ***Engine efficiency***
- ***System integration***
- ***Tires***
- ***Weight***
- ***Aerodynamics***

How do we improve fuel efficiency?



Adapted from David Foster (UW), Transportation Combustion Engine Efficiency Colloquium, March 3 – 4, 2010

Heat transfer:

Flow
- Mean flows (Swirl, Tumble)
- Turbulence

Temperature & Composition
- CR
- Lambda
- EGR
- Comb. Phasing/Duration
- Soot radiation

Geometry
- Chamber shape, B/S

Exhaust losses:

Work Extraction
Comb. Phasing/Duration

Charge composition (lean, EGR

Linked to heat transfer
(interacts with gas properties to impact work extraction!))

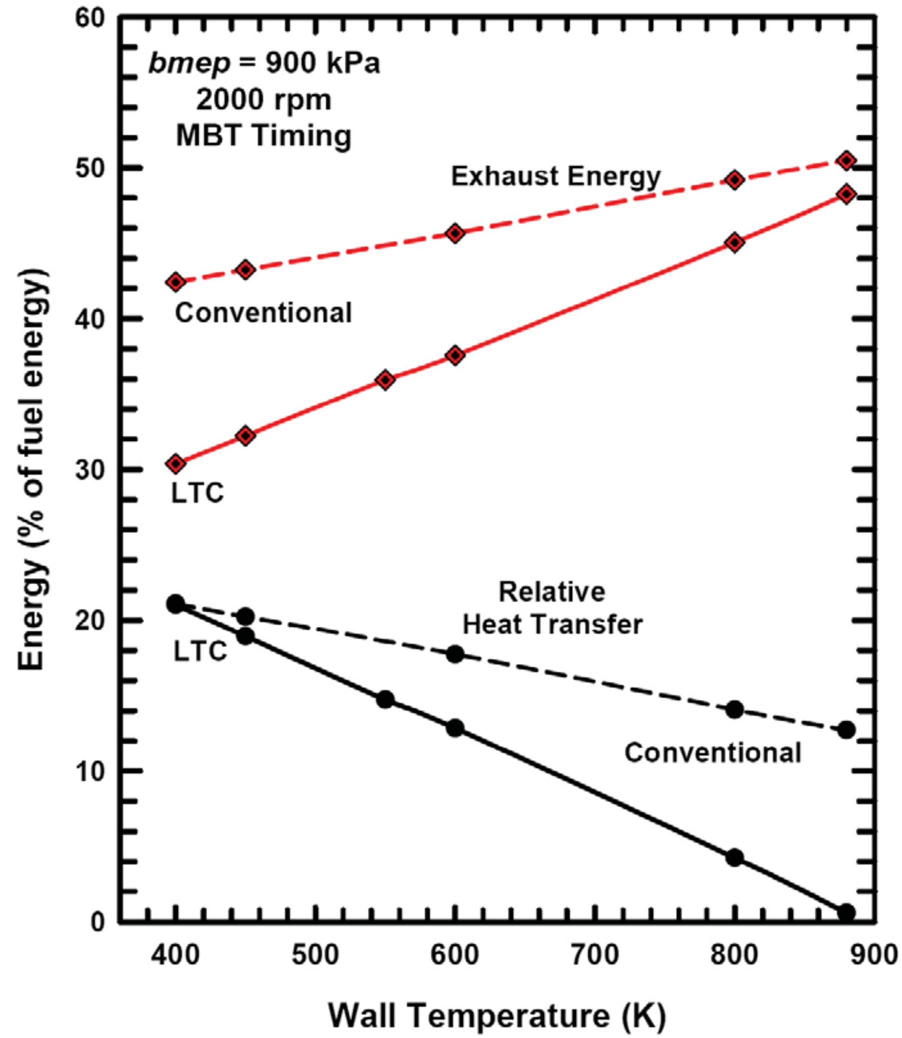
Why didn't "adiabatic" engines deliver on the promise of increased efficiency?

- For conventional diesel combustion, increased wall temperature increases the exhaust gas energy by ~ the same amount as the heat transfer is reduced

  (reduced γ with higher temperatures decreases the ability to extract work by expansion)

- For low-temperature combustion, the increase in exhaust energy is less that the reduction in heat transfer
  - a greater reduction in heat transfer is observed under LTC conditions
  - a greater increase in exhaust energy is also observed, but more work is extracted due to higher γ

Source: SAE 2011-01-0312



Principal challenges*: Integrated fuel injection and spray models

"Mixture preparation & combustion begins with the introduction of fuel"

- Robust, grid-independent engineering design codes needed to capture:

  Internal nozzle flow phenomena:

  - Cavitation
  - Wear
  - Structural interactions

  Coupling to external flow:

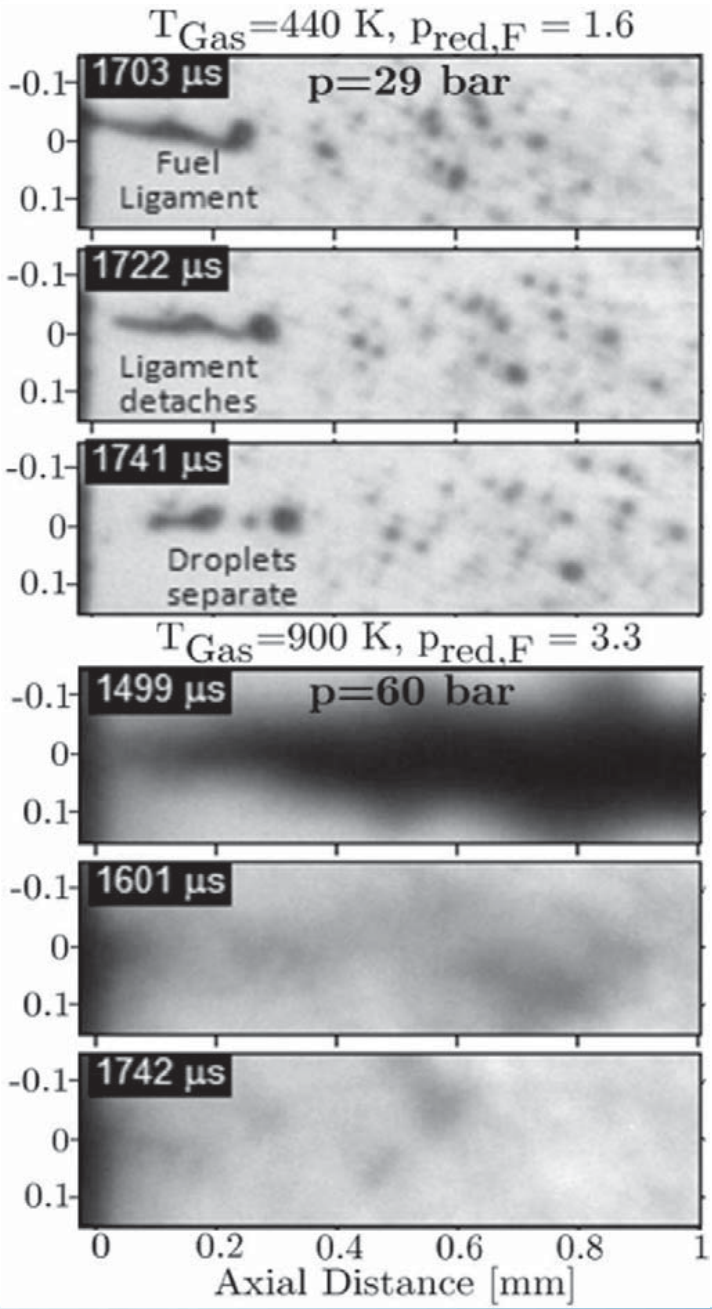
  - Flash boiling
  - Primary and secondary break-up mechanisms
  - Spray penetration
  - Droplet size distributions
  - Droplet-gas momentum transfer
  - Droplet interactions with turbulence field
  - Multi-component vaporization
  - Modeling for trans/super-critical conditions

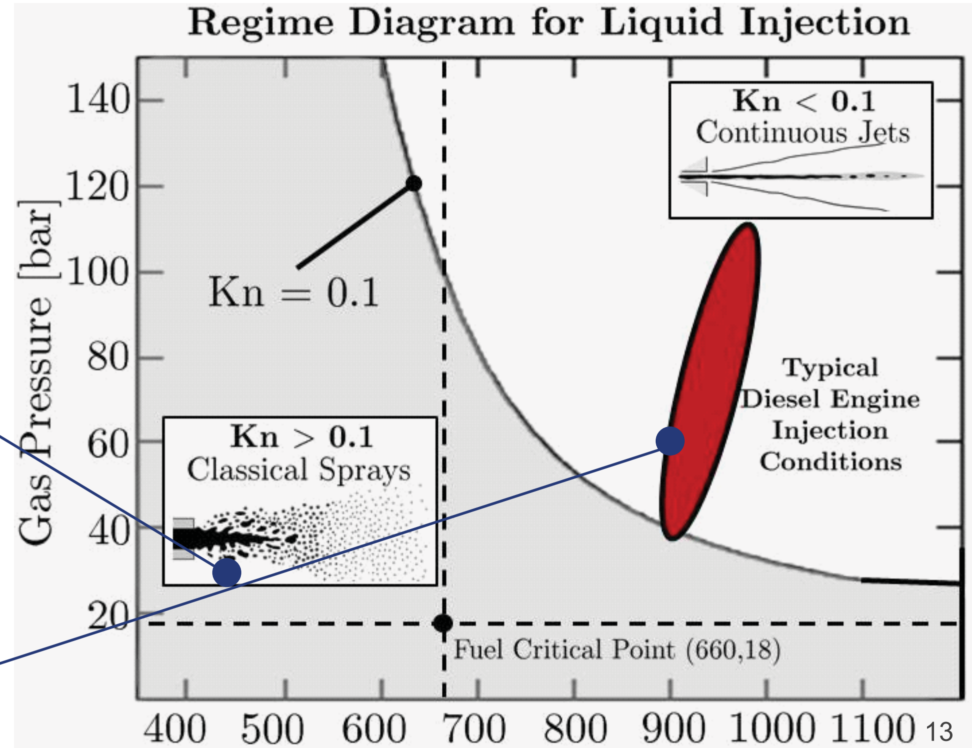
- Experimental validation data needed:
  - High-speed, high-resolution measurements of spray structure in the near-nozzle region
  - Impact of atomization regime on subsequent entrainment and mixture preparation;
  - In-nozzle flows and cavitation

- Many models will need to be developed from high-fidelity simulations (LES, DNS)

* Draws heavily on industry input to the DOE PreSICE workshop, March 3, 2011

Spray models may be strongly dependent on the specific thermodynamic conditions





- At lower temperatures and pressures, discrete ligaments and droplets are observed
- A higher pressures and temperatures only diffuse interfaces are observed
- Model development will likely require both simulations and experiments
- Imaging techniques require refinement

Principal challenges: Flow Modeling

"Fluid mechanics is the foundation of mixture preparation & combustion"

Accurate, massively-parallel, robust CFD codes must:

- Capture cycle-to-cycle fluctuations and associated stochastic events (misfires, pre-ignition – implies LES)
- Efficient codes for steady flows and parameter optimization – implies RANS
- Mesh with CAD input / on-the-fly mesh generation (geometry optimizations)
- Accurate numerics with well-understood mesh & time step dependence
- Realistic wall treatments
- Single code for all applications (LES, RANS, SI, CI) desirable

Validation will be a challenge – moving beyond simple statistics

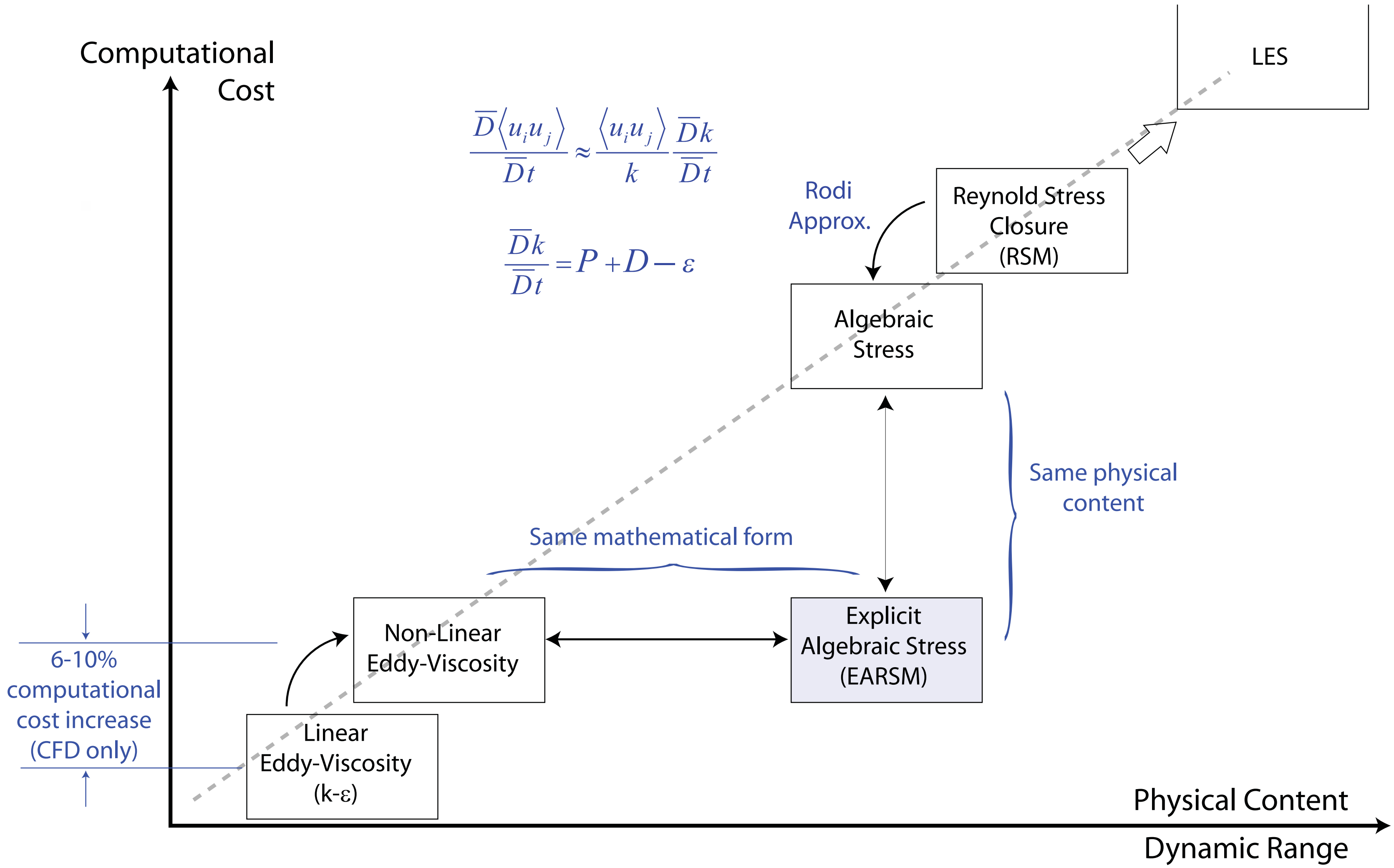
- Cycle-resolved measurements of flow structure, mixture distribution, ignition, and pollutant formation required

Modeling efforts will be central the improvement of RANS-based codes

- Models will need to be developed from high-fidelity simulations (LES)

Computational cost and physical content are not perfectly correlated

Graph adapted from Gatski & Jongen
Prog. Aero.Sci. 36 (2000):655-682

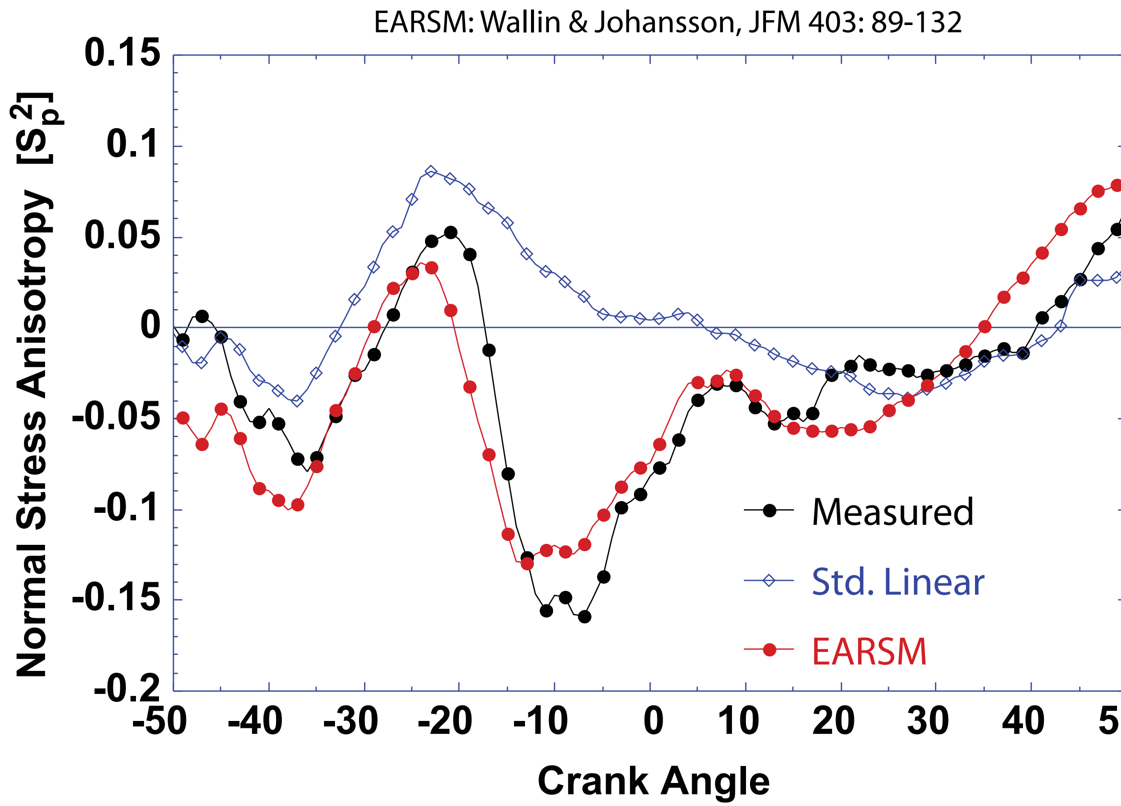


The "best" model is one which provides sufficient accuracy at the most economical cost. A heirarchy of models or approaches is needed

Non-linear, EARSM-based relationships can significantly improve predicted turbulent stresses

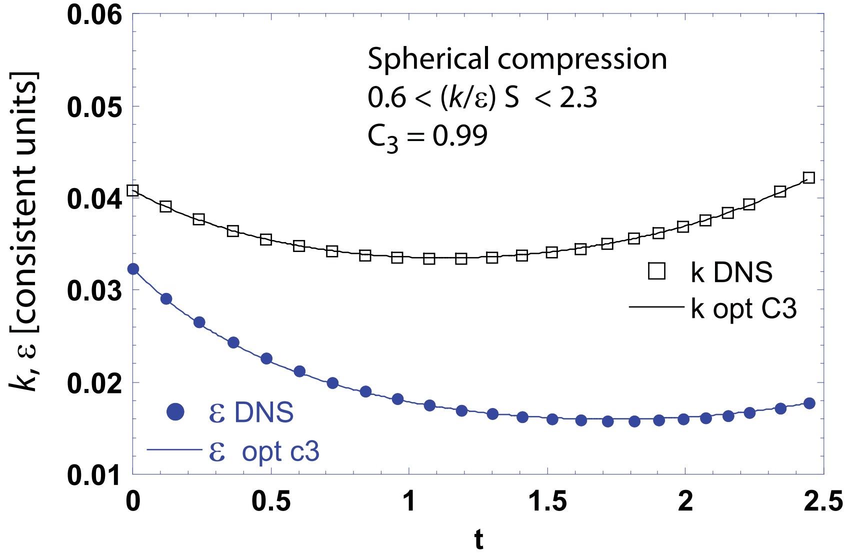
$$\frac{\langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij}}{2k} = -C_\mu \left(\frac{k}{\varepsilon}\right) S^*_{ij}$$

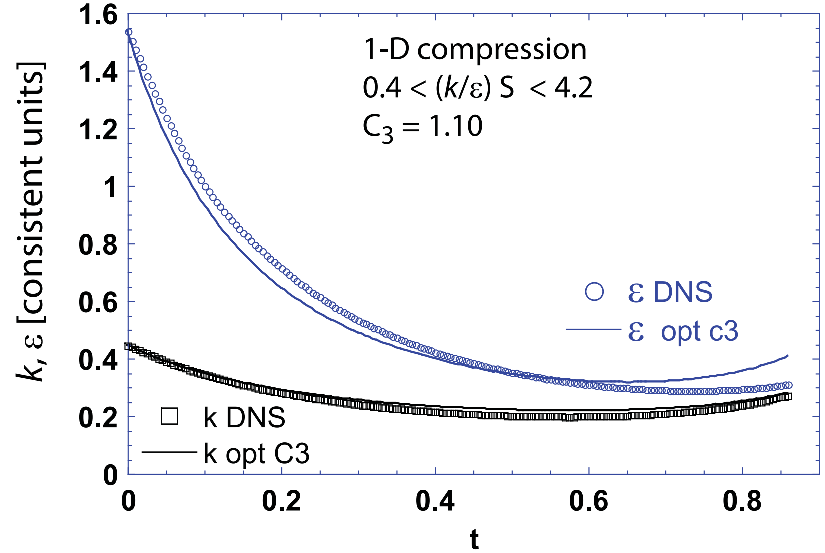
$$+\alpha_2 \left(\frac{k}{\varepsilon}\right)^2 \left(S^*_{ik}\Omega^*_{kj} - \Omega^*_{ik} S^*_{kj}\right)$$



- The standard linear stress relationship fails profoundly
- The EARSM-based stress relationship s a significant improvement
- Re-distribution physics are retained

Direct numerical simulation (DNS) can resolve long-standing issues in the modeling of C_{ε_3}





$$\frac{D\varepsilon}{Dt} = C_{\varepsilon 1}\frac{P\varepsilon}{k} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} + (1 - C_{\varepsilon 3})\,\varepsilon\,(\nabla\cdot\mathbf{U}) + \text{Diffusion}$$

- The k and ε equations, with standard values for the coefficients C_{ε_1} and C_{ε_2}, can match the DNS predictions well with $C_{\varepsilon_3} \approx 1$ (Strain dependent coefficients may help further)
- The DNS results were obtained at very low Re ~16; compression times are small compared to ℓ/u'

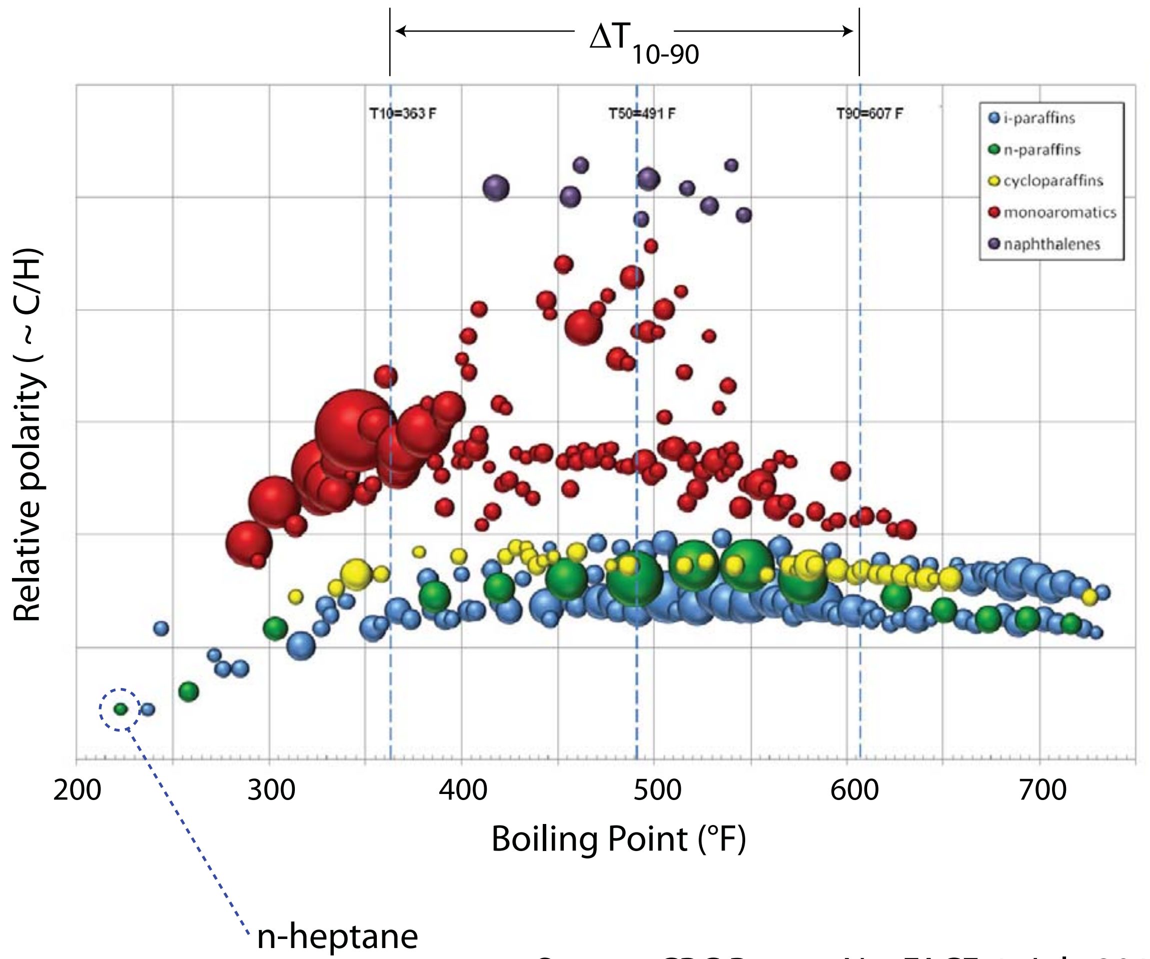
RANS turbulence modeling could benefit from fundamental DNS studies with modern computing capacity

Principal challenges: Multi-component kinetics

"Kinetics impact both auto-ignition and flame propagation processes "

- Diesel fuel is an enormously complex mixture of compounds with vastly different physical and chemical properties
- Most simulations of diesel combustion are currently performed using kinetic mechanisms developed for n-heptane

How can we realistically handle the kinetics of real fuels?

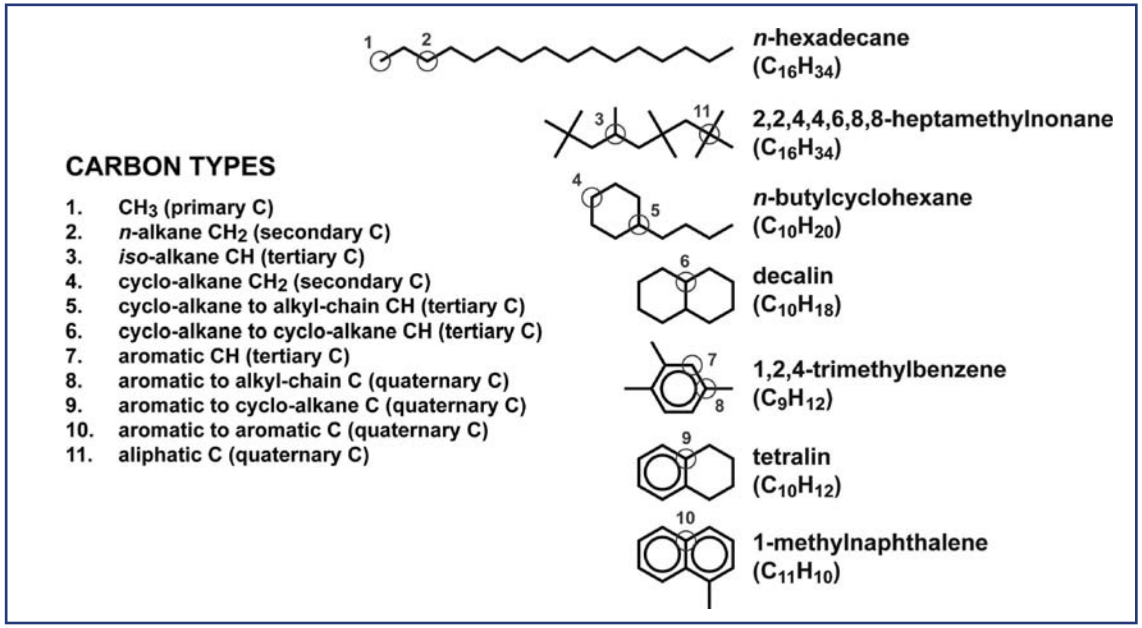


Source: CRC Report No. FACE-1, July 2010

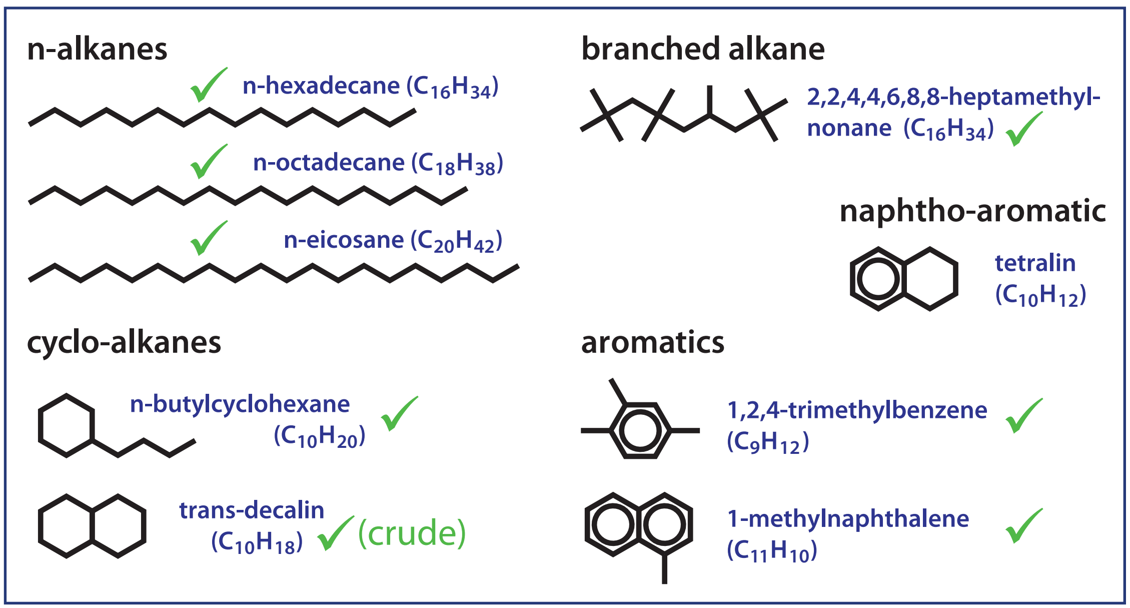
Acknowlegement: Chuck Mueller, Sandia

Considerable progress has been made in defining appropriate surrogate fuels

- Carbon bond types, physical properties, and autoignition characteristics are considered to define a "pallette" of surrogate fuel components



Pallete:



- Validated kinetic mechanisms are available for several of the pallete compounds (✓)
- Regression analysis can be used to adjust the fraction of components from the pallete to best match specific fuel types

Sources: Energy & Fuels 26: 3284, 2012
WJ Pitz, DOE Merit Review 2013

Principal challenges: Wall interactions

"A significant fraction of the fuel energy is lost to heat transfer"

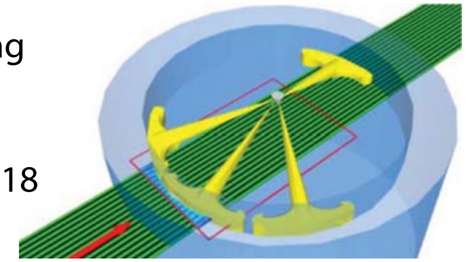
- Heat transfer is poorly understood in engines

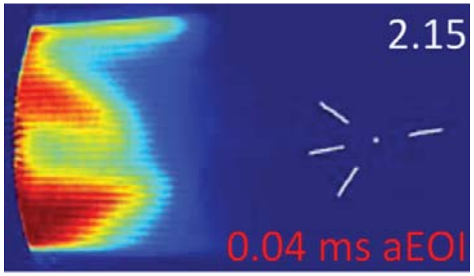
  Law-of-the-wall based formulations for velocity & temperature boundary layers are:

  - Inconsistent with transient nature of engine flows
  - Inconsistent with compressible turbulence models
  - Reported to fail in swirling flows
  - Not validated on a detailed level

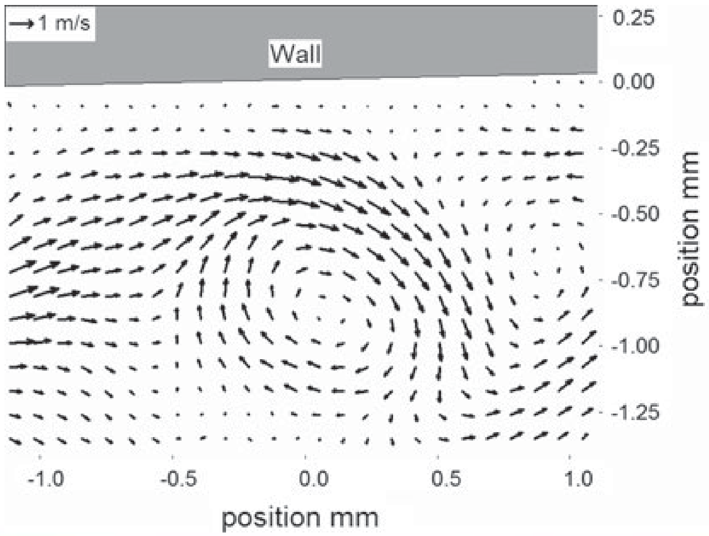
- Advances in measurement techniques and high-resolution near-wall measurements are becoming available, but more are needed
- Wall interactions also include spray interactions, film formation and vaporization
- Model development will benefit greatly from high-fidelity simulations (LES, DNS)

Near-wall ϕ using structured-illumination SAE 2012-01-1718





High-Resolution PIV: Exp. Fluids 49: 949 (2010)



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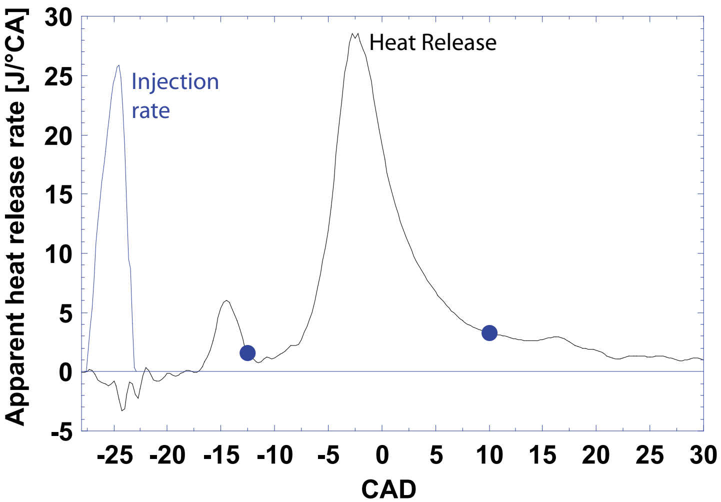
Qualitative PLIF imaging of D2 suggests discrete droplets are formed from piston-top films:

-12.5° aTDC

10° aTDC



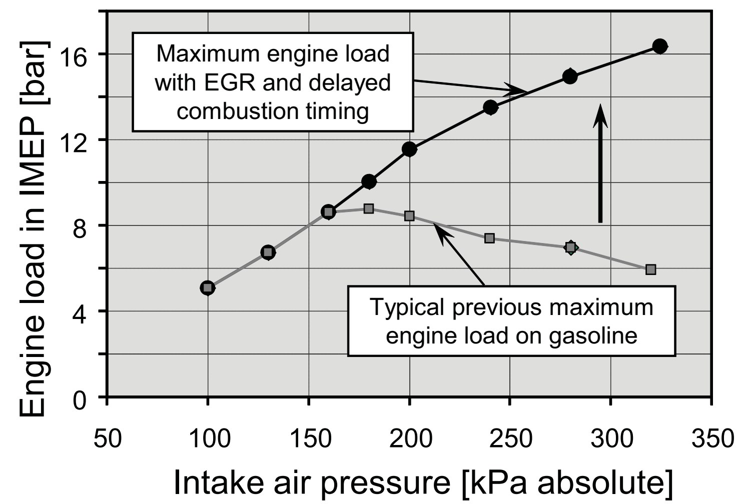
Principal challenges: High-pressure, dilute combustion

"High-pressure, dilute combustion processes are key to high power density, high efficiency, low-emission engines"

- With sufficient boost, high HCCI power densities can be achieved with very low emissions
  - 87 octane gasoline
  - No knock, stable combustion
  - Ultra low NO_x / soot
  - 47-48% indicated efficiency over 8–16 bar IMEP

  High pressure ignition chemistry of gasoline-like fuels is still not adequately captured

Acknowledgement: John Dec, Sandia



- "HEDGE" combustion, "PREMIER" (natural gas) combustion

  Runs close to knock – transition to & mechanism of rapid latter burn not understood

- Models for dilute combustion must have well-understood range of applicability (premixed through mixing-controlled; flame propagation through autoignition); require little user knowledge of combustion regimes

Additional Challenges

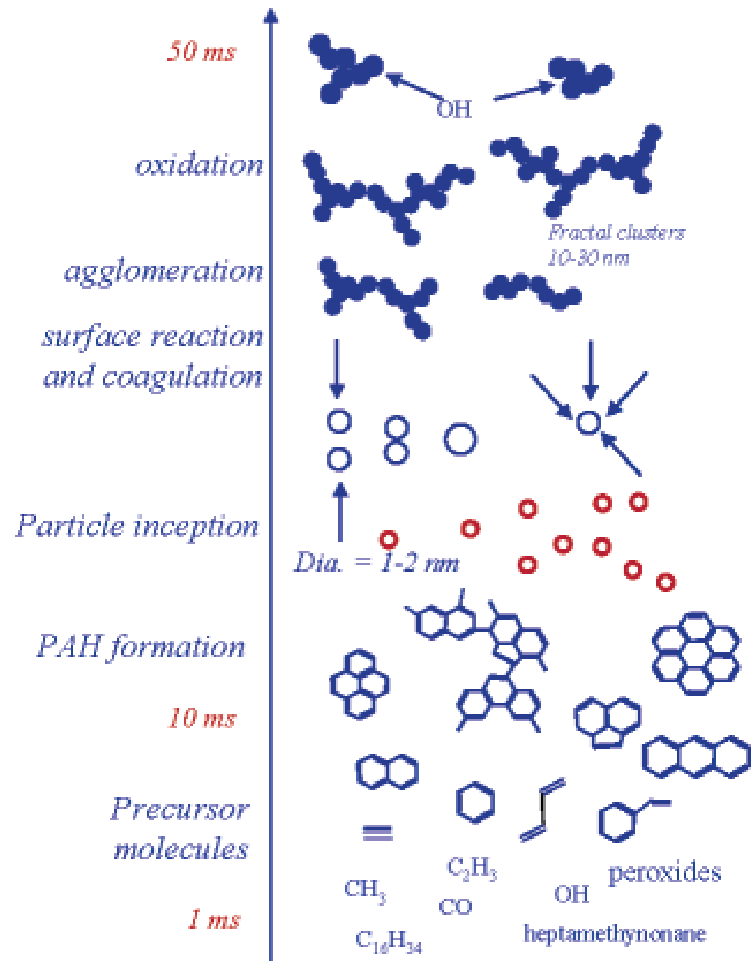
Heterogeneous Chemistry

- Soot modeling

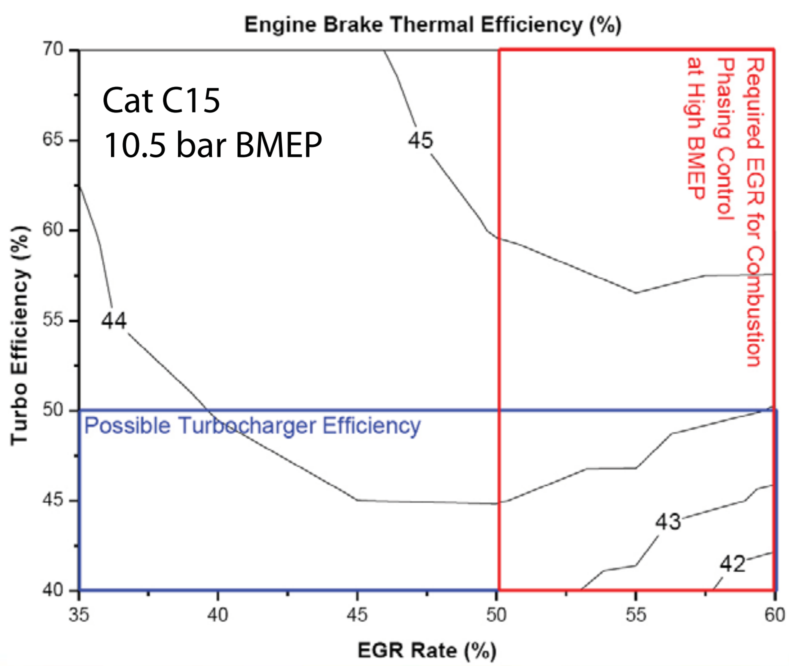
  Soot particle number now regulated

- Surface chemistry and physics

  Critical for low-temperature catalysis, filter regeneration



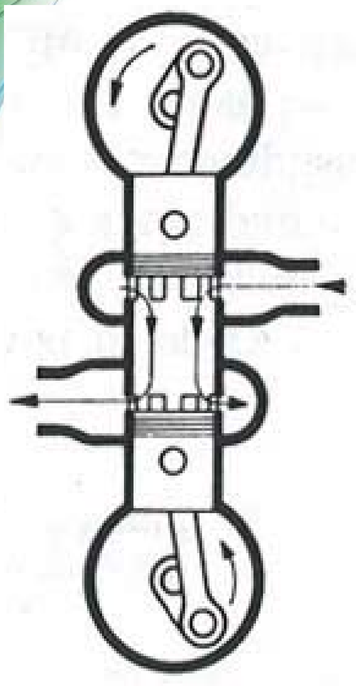
Source: J. Chem. Theory Comput. 2:504 (2006)

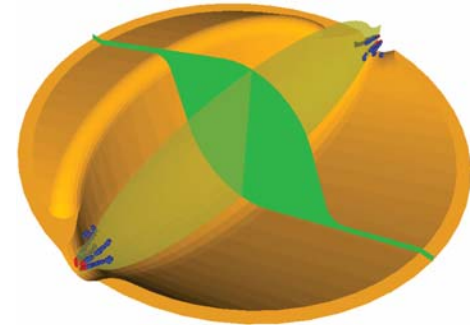


- Turbocharger / Air handling technology

  Limits practical application of high-efficiency combustion techniques

Alternative engine architectures offer a promising path forward



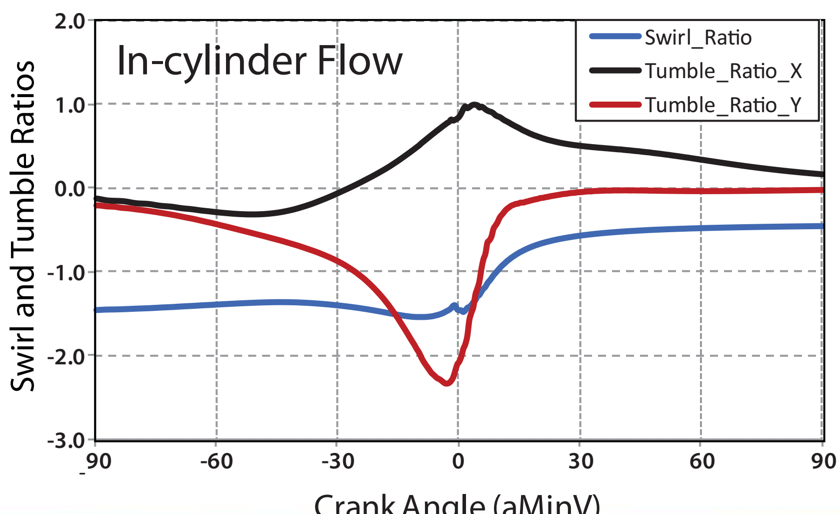


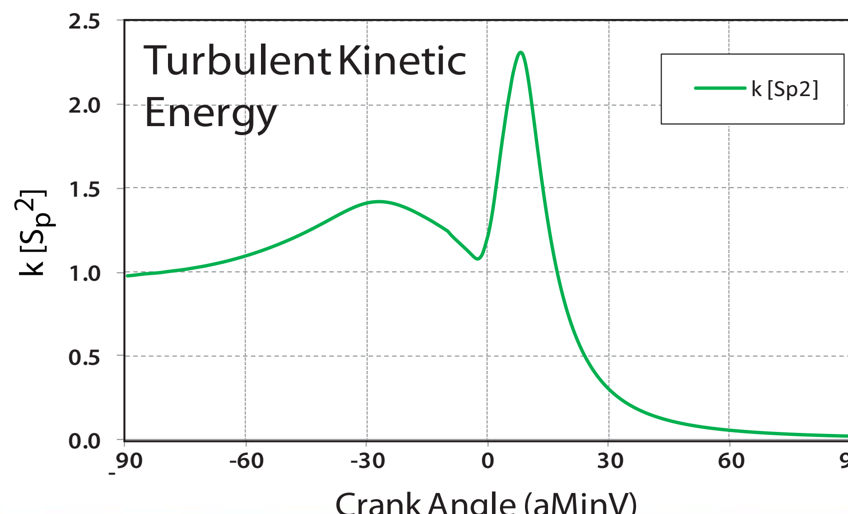
Example: Achates Power 2-Stroke Engine

Opposed piston, ported architecture permits design flexibility not possible with poppet valve architectures

Heat transfer and exhaust enthalpy losses addressed by:

- Reduced combustion chamber surface area
- Combustion and in-cylinder flow control
  - Unique piston shape promotes strong tumble motion and breakdown
  - High near-TDC turbulence levels promote rapid burn
  - Turbulence, swirl, and tumble rapidly attenuated during expansion





A 20 year perspective...

- IC Engines will remain the dominant transportation powerplant
- Increased fuel efficiency (low CO_2 emissions), with criteria emissions compliance, will be a major driver for engine design
- Engine design *and calibration* will be largely performed via simulation, with limited testing for confirmation
- Alternative engine architectures will penetrate niche markets (where fuel efficiency is king and packaging constraints less severe)
- Experimental capabilities will allow detailed 3-d measurements of flow and scalars

  Near-wall and high pressure/temperature techniques will advance

  High-accuracy, high spatial- and temporal-resolution measurements (i.e. small-scale turbulence) will remain challenging)
- Simulation capabilities continue to advance, driven by advances in numerics, more efficient modeling, and hardware advances

  Direct simulation of spray break-up processes in sight

  LES-based design tools will be used to design for minimal cyclic variability

  RANS-based tools will remain important for optimization and calibration

Expectations of exponentially increasing computing power should be viewed cautiously

- Increased semiconductor feature density will not continue indefinitely

  Vertical integration, multi-state logic, "More-than-Moore" diversification, non-silicon extensions will all help

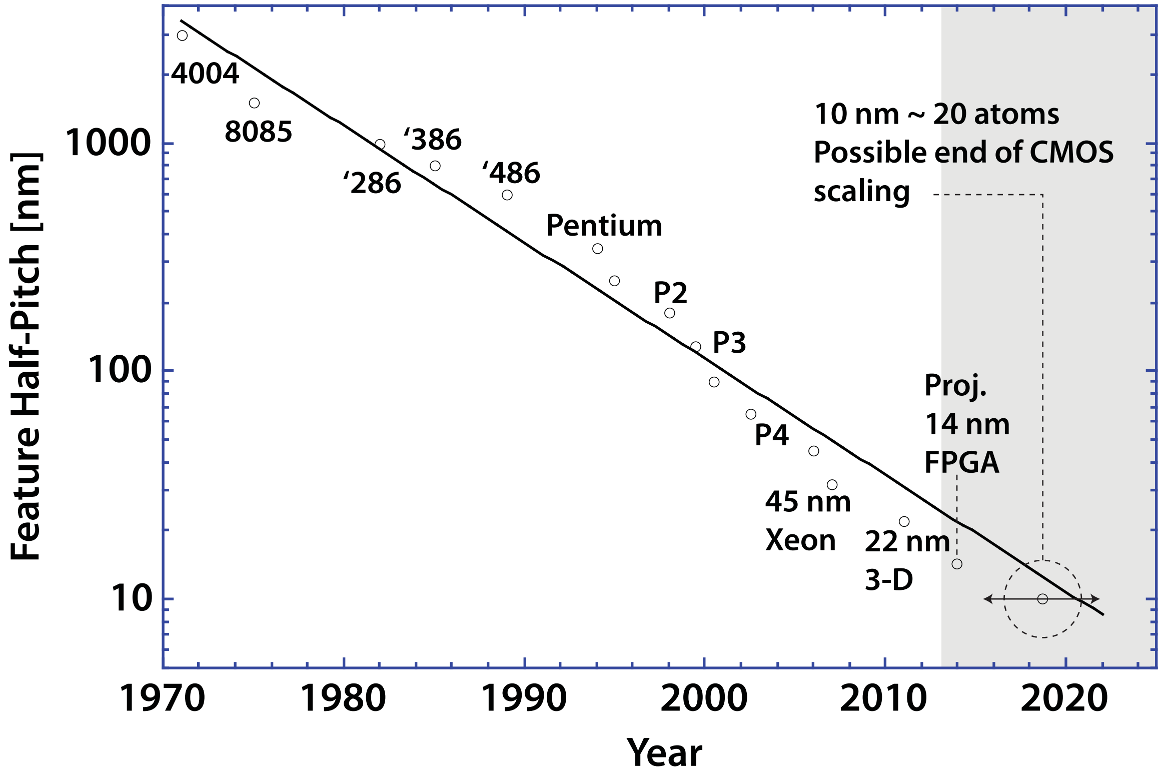
  Some argue 'no-limit' to scaling

- Low power solutions will be essential

  Thermal management

  Cost (~ \$20M/yr electricity for exaflop computing)

Moore's law:



Modeling – and subsequent implementation into lower computational cost design tools – will be part of a balanced research portfolio