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Pathways to Science-Based Combustion Technology

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Outline of presentation

- Technology drivers
- Combustion science: progress and challenges
- Technological progress through inter-disciplinary collaboration
  - Case study: engines
  - Computational modeling: status and prospects
  - Implications of alternate fuels
- A concept that connects
  - Spray combustion
  - Lifted turbulent diffusion flames
  - Char oxidation
  - Coal pyrolysis
  - Solid-propellant combustion
- Perspective

Combustion science is guided by technology issues, and is largely empirical

Key questions:

- Does the mixture burn?
- What is the burning rate?
- What is the efficiency of delivery of desired outputs? (e.g., mechanical work, heat to load)
- What are the chemical products?

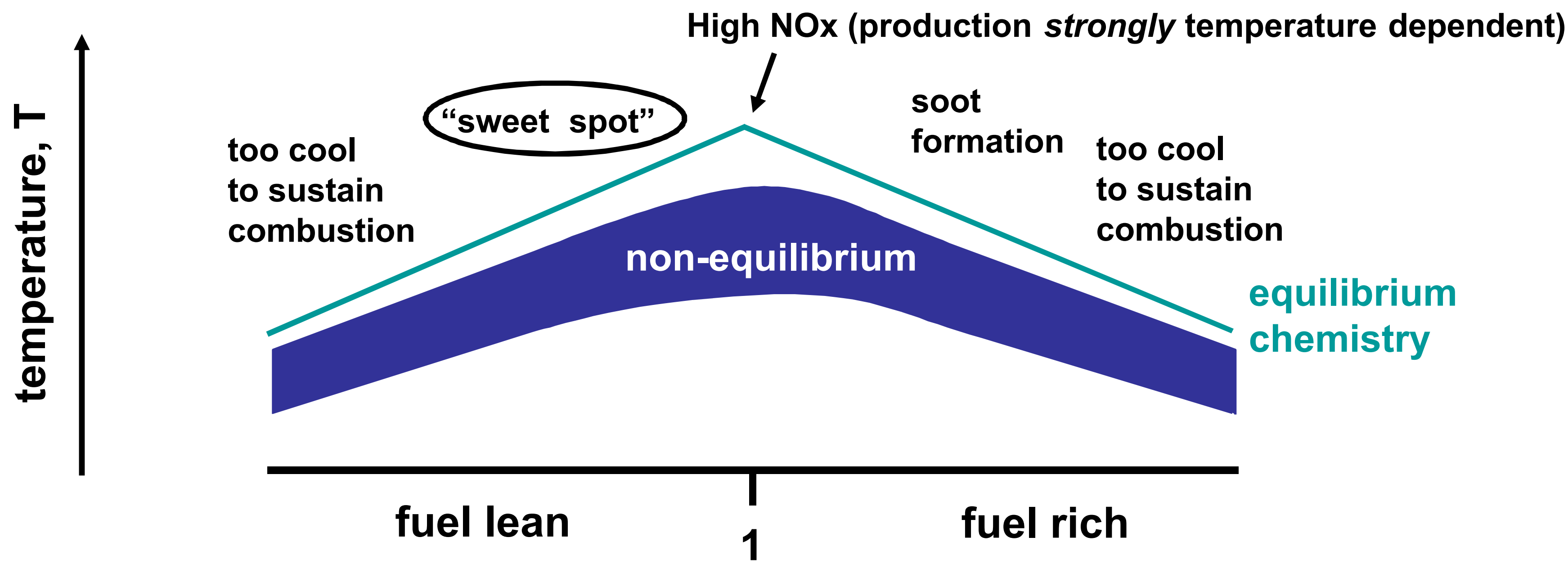
Premixed and non-premixed flames are dynamically distinct

- Premixed combustion
  - fuel-air mixture of uniform composition
  - flame speed is controlled by chemistry and heat transport
  - burning rate is flame speed times surface area
  - fluid turbulence increases surface area, hence controls the burning rate

- Non-premixed combustion
  - flame resides on (or near) the surface of fuel-air stoichiometry
  - reaction rate is controlled by transport that mixes fuel and air
  - turbulence controls the mixing rate

The intermediate case, 'partially premixed combustion,' is scientifically challenging and technologically important

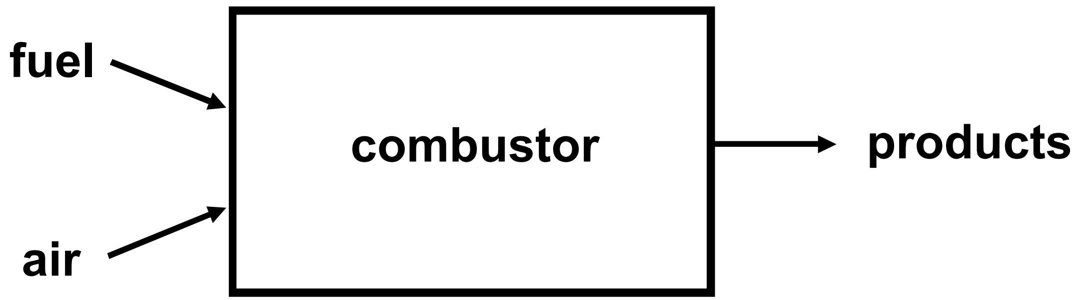
The *equivalence ratio* governs flammability and chemical product yield



Equivalence ratio, **Φ (fuel-air ratio relative to stoichiometric)**

Pollutant minimization motivates combustor operation near the *lean flammability limit*

Maximization of the burning rate motivates operation near flame extinction



- High throughput requires short residence time
- To avoid extinction ("blow-out") this time must not fall below chemical time scales
- Near-extinction operation requires control, and understanding, of flow-chemistry interactions

Combustion is one of many drivers of device design

- Materials must withstand combustion temperatures and temperature variability
- Device geometry and operation must avoid instabilities that
  - cause catastrophic failure
  - reduce service life
  - produce unacceptable noise
- On-board mixture preparation and ignition is usually needed
  - Spray formation (carburetor, injector) and vaporization
  - Spark, glow plug, pilot flame, plasma torch, compression ignition
- Mitigation strategies can ease constraints
  - catalytic conversion of NOx
  - carbon sequestration

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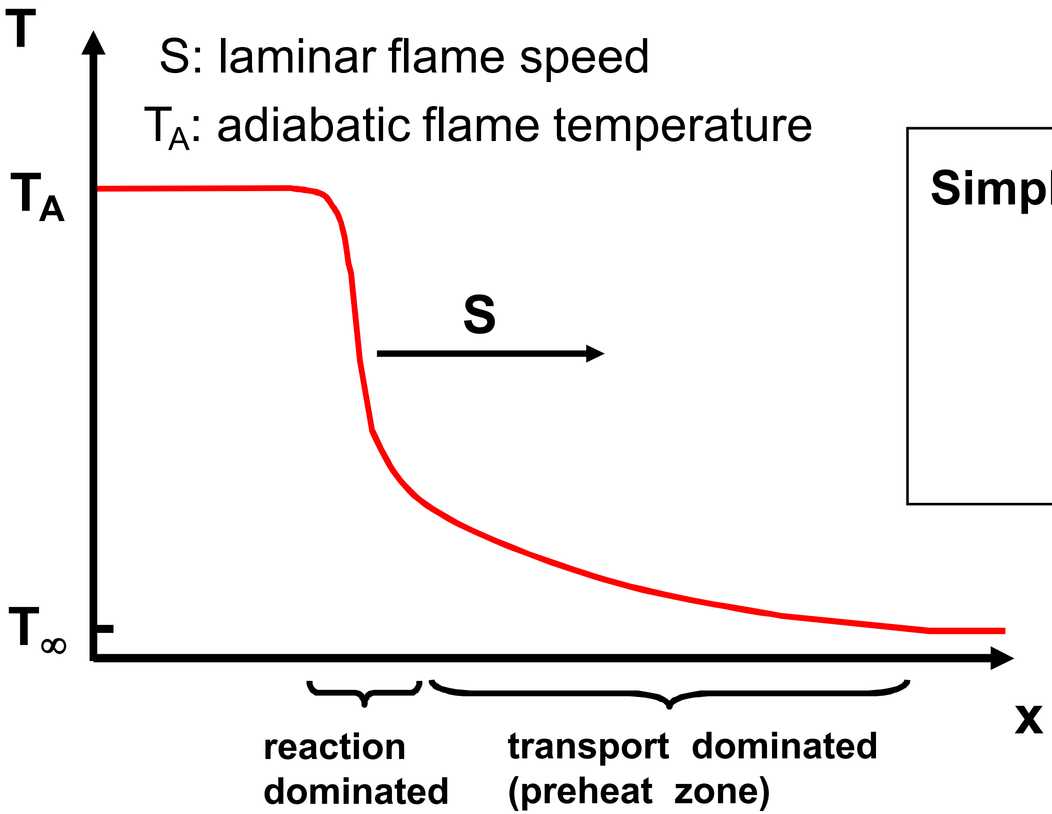
The simplest premixed flame idealizations raise non-trivial math and physics issues



Simplifying assumptions:

- Steady flame propagation
- Constant density
- No fluid motion

progress variable:

$$c \equiv \frac{T - T_\infty}{T_A - T_\infty}$$

evolution equation:

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} + f(c)$$

The governing physics depends on the functional form of the reaction-rate term *f(c)*

evolution equation: $$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} + f(c) \qquad c(\infty) = 0; \quad c(-\infty) = 1$$

For $f(c) = c(1-c)$ (Fisher equation) and other convex f with $f(0) = f(1) = 0$,

the Kolmogorov-Petrovskii-Piskunov (1937) ***velocity selection principle*** implies

$$S = 2\left(\kappa \left.\frac{\partial f}{\partial c}\right|_{c=0}\right)^{1/2}$$

depends only on the earliest onset of reaction

For combustion, f peaks sharply near $c = 1$ and is nonzero at $c = 0$, e.g.

$$f = (1-c)\exp\left(-\frac{E_A}{RT}\right)$$

In this case, ***activation-energy asymptotics*** (Bush & Fendell, 1970)

shows that S depends on properties of f near its peak.

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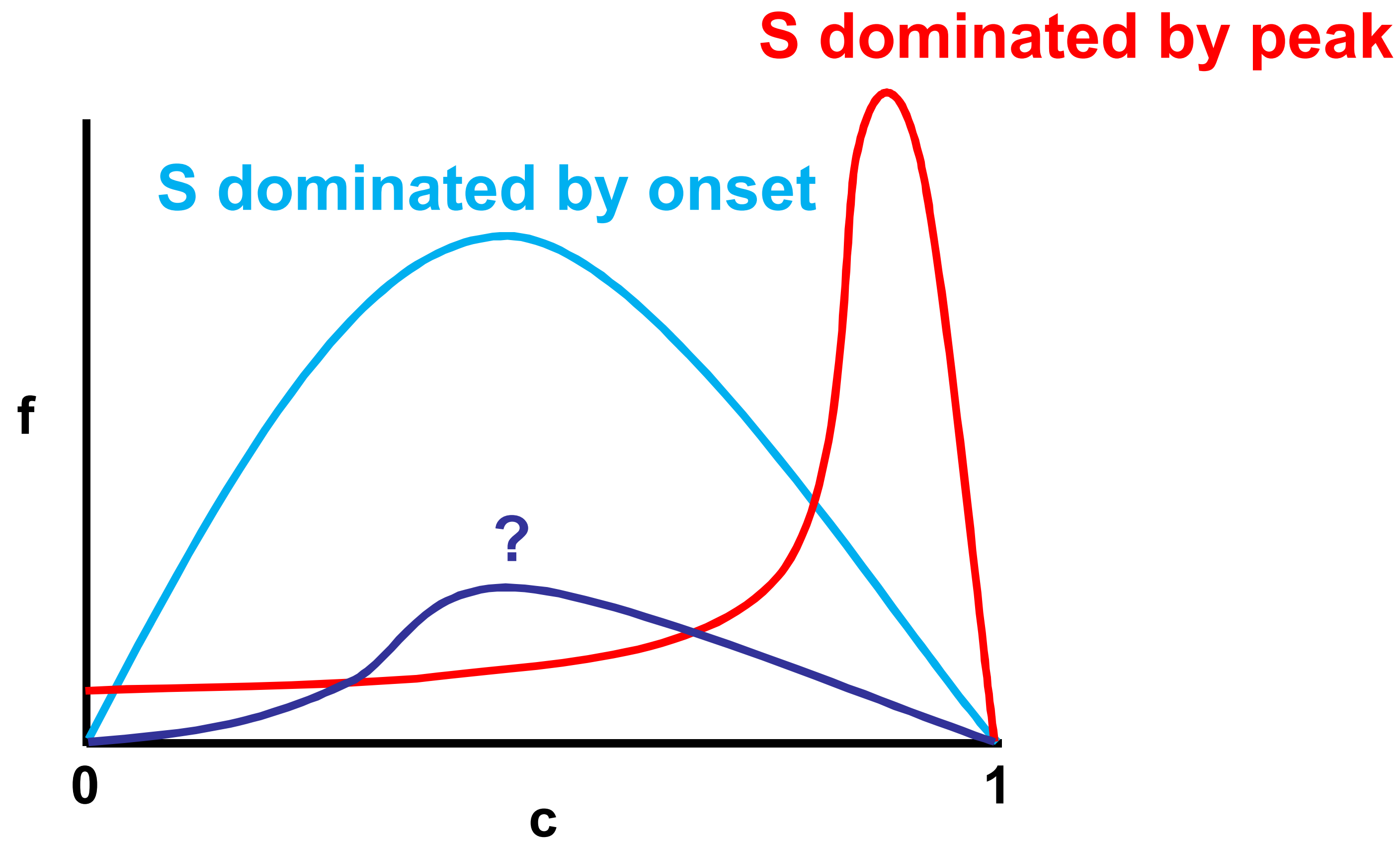
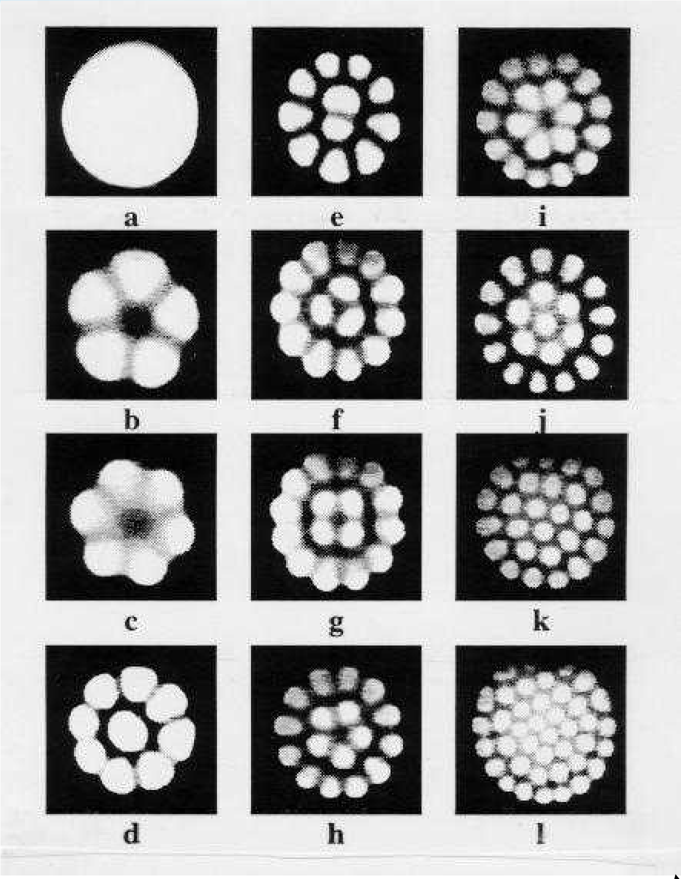
Are there other physically relevant diffusion-reaction regimes?



Real flames are subject to instabilities



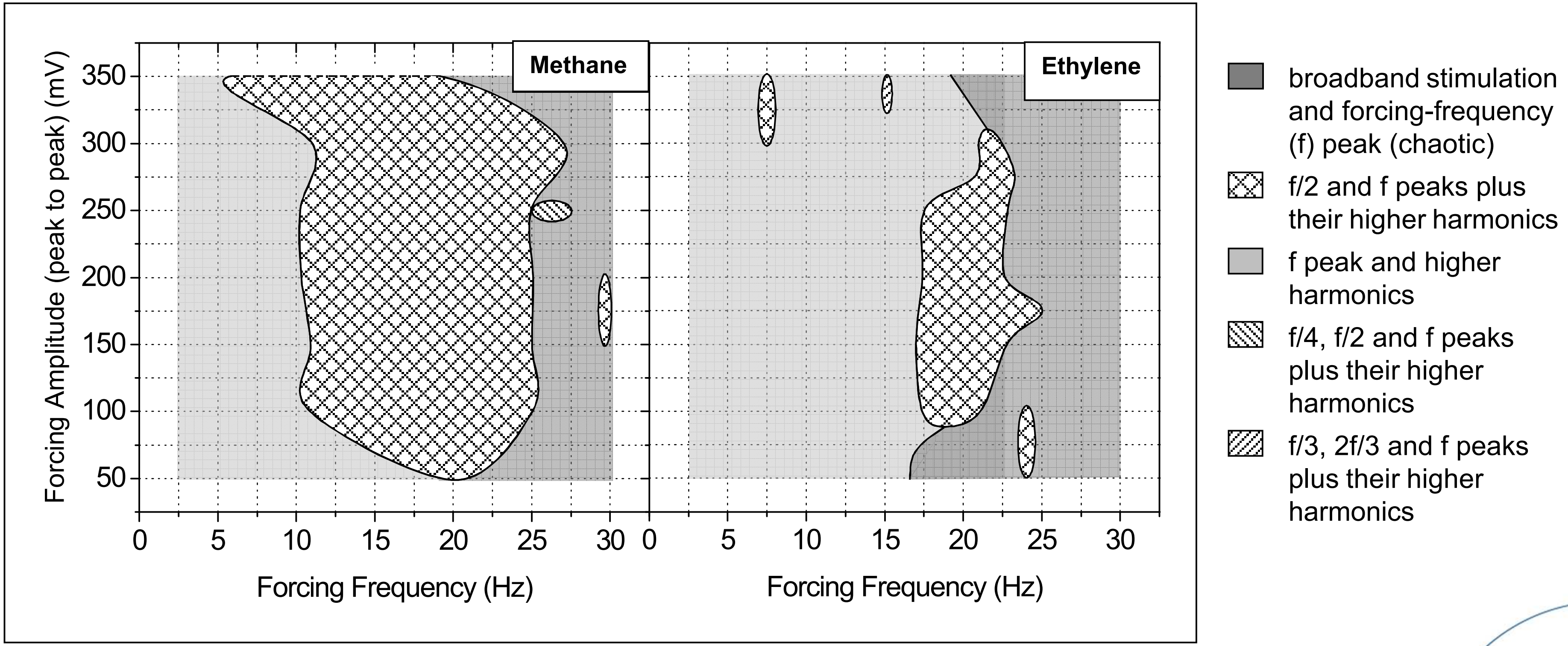
theory cannot identify the instability mechanism

Sequence of cellular instabilities on a flat burner (Gorman, el-Hamdi, and Robbins, 1994)

- Hydrodynamic instability (due to unequal fuel and product densities)
- Diffusional instability (due to unequal heat and species diffusivities)
- Instabilities can be
  - steady (e.g., cellular)
  - time-periodic
  - chaotic
- Much of this physics is captured by the *Kuramoto-Shivashinky equation*

Flames exhibit dynamical complexity that is not yet understood

Spectral response of line-of-sight luminosity to acoustic forcing of a buoyant non-premixed flame (Williams, Shaddix, and Desgroux, 2003)



The joint PDF of T and species is used to model turbulent non-premixed combustion

thermochemical state:

$$\vec{c} = (c_1, \ldots, c_{N+1})$$

N species concentrations + temperature, assuming constant pressure

chemical evolution:

$$\frac{\partial c_i}{\partial t} = f_i(\vec{c})$$

omits advection and diffusion

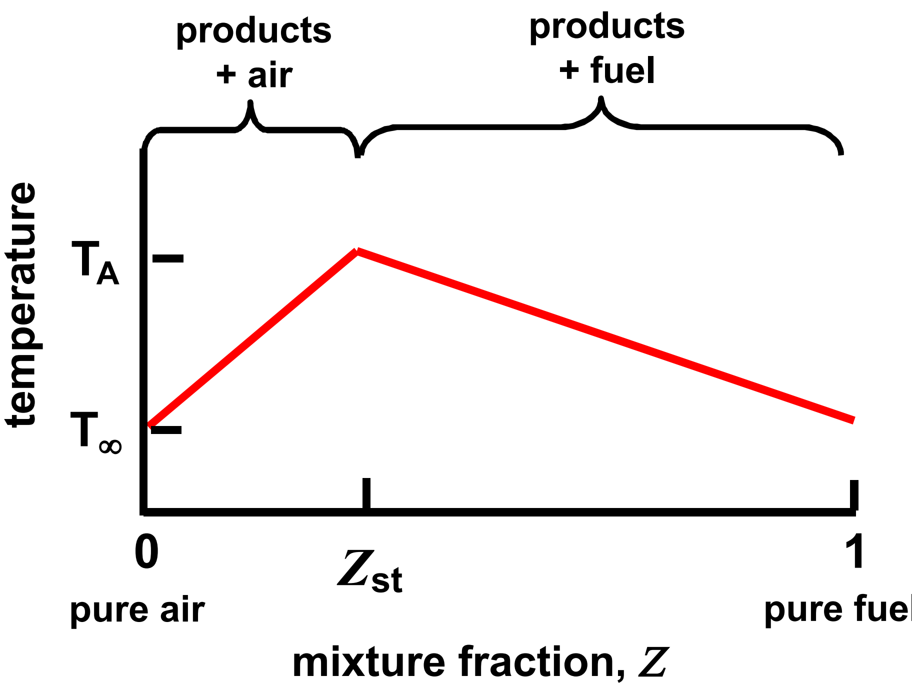
mean chemical evolution:

$$\frac{\partial \langle c_i \rangle}{\partial t} = \int f_i(\vec{c}) g(\vec{c})\, d\vec{c}$$

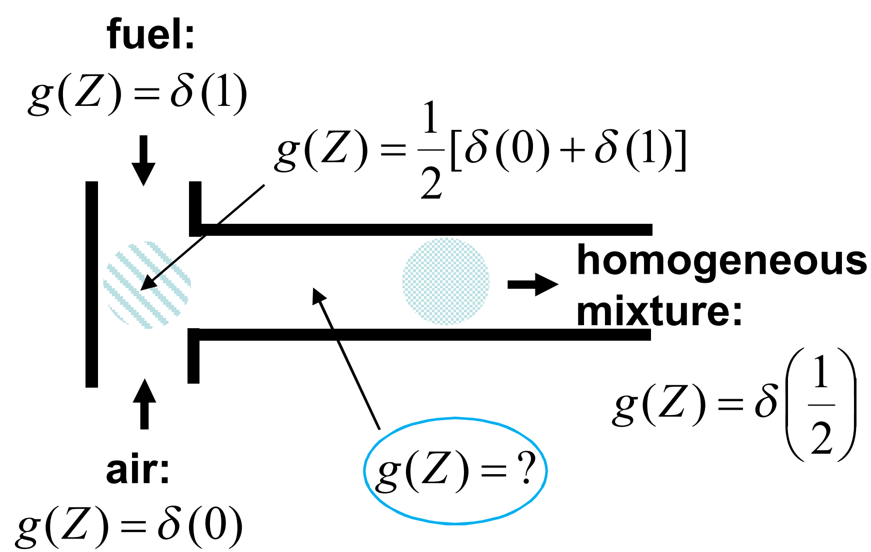
where $g(\vec{c})$ is the joint PDF of state variables

For two-stream (e.g. fuel-air) mixing, the mixture-fraction PDF is often sufficient

For fast chemistry (relative to mixing), the mixture fraction *Z* determines the (equilibrium) chemical state



The combustion problem is thus reduced (under certain approximations) to a passive mixing problem



Need to predict:	• Sequence of mixture-fraction PDF shapes $g(Z)$ • Rate of evolution through shape sequence

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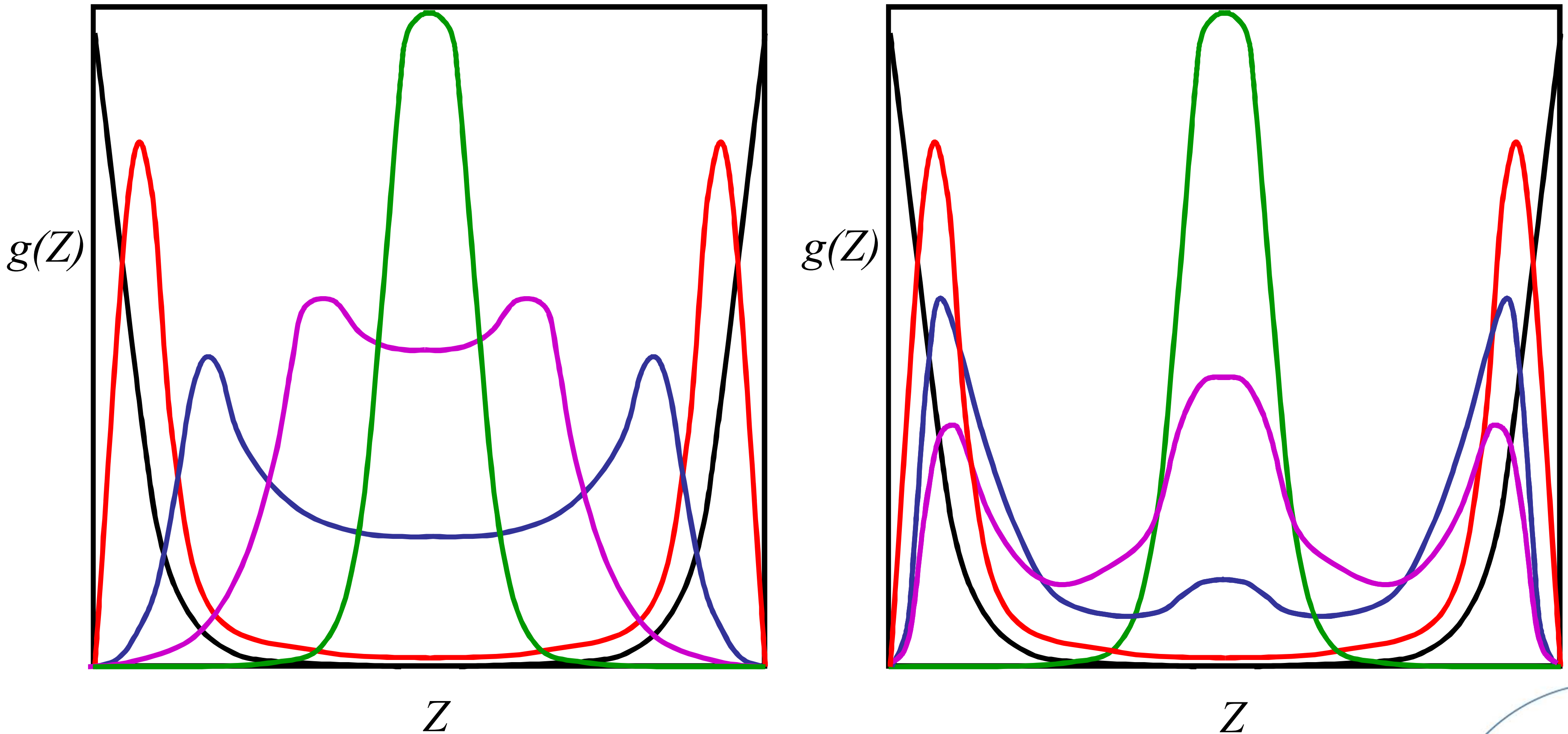
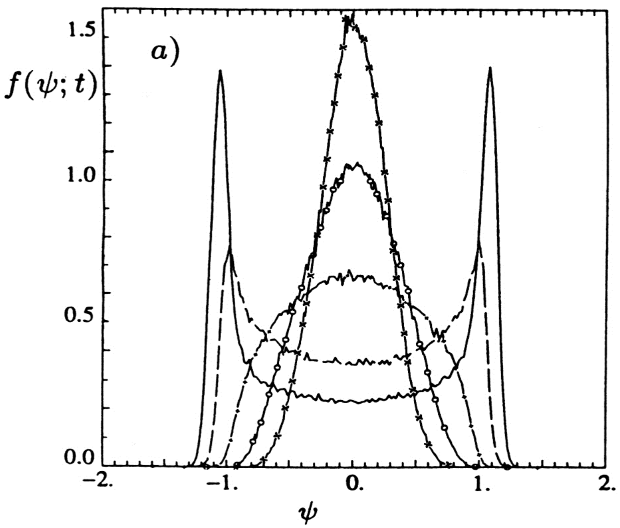
Several distinct PDF evolution scenarios are possible

$1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5$

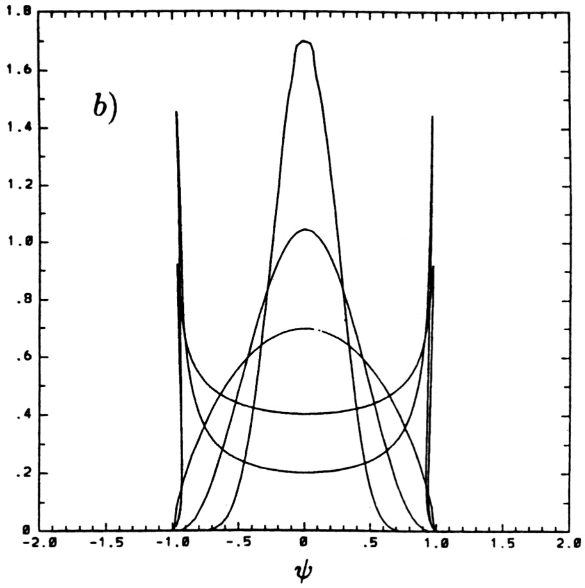


An observed PDF sequence is remarkably well reproduced by a simple model

direct numerical simulation (Eswaran & Pope 1988)



mapping closure (Pope 1991)



What is the significance of this comparison?

The agreement of mapping closure with DNS is impressive but puzzling

- Method (Chen, Chen, & Kraichnan 1989; Pope 1991)
  - Define a function $Z_G(Z)$ such that the PDF of Z_G becomes Gaussian
  - Simple assumptions give an evolution equation for $Z(Z_G)$
  - The flow field affects the mixing rate but not the PDF shape sequence
- Issues
  - Does the mapping closure analysis capture mixing physics?
  - The flow field and initial Z field can be manipulated to generate diverse PDF sequences - what is special about the DNS PDF sequence?

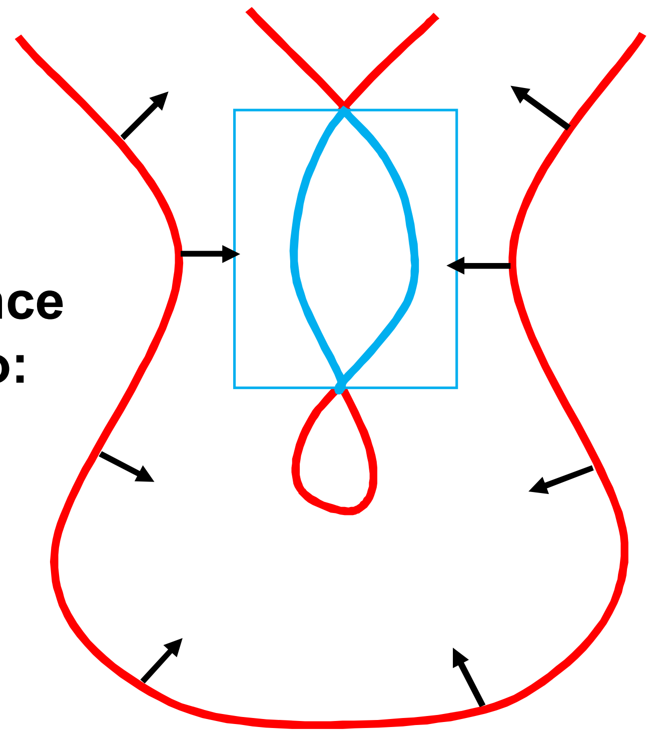
Idealization of turbulent premixed combustion: passively propagating advected interface

- Constant propagation speed $\boldsymbol{S}$, constant density
- Turbulence characterized by RMS velocity fluctuation $\boldsymbol{u'}$
- For $\boldsymbol{u'}$ dominance ($\boldsymbol{u'} \gg \boldsymbol{S}$), the burning velocity $\boldsymbol{v}$ (volumetric fuel-consumption velocity) scales as $\boldsymbol{u'}$
- Interpretation: turbulent entrainment rather than burning is rate limiting

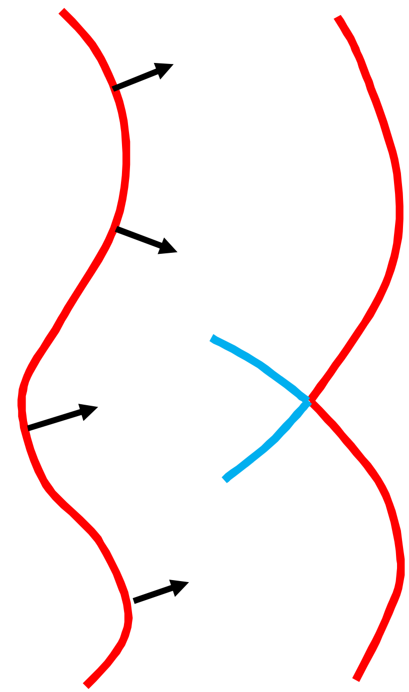
Progress beyond this level of analysis is mainly empirical

Flames stretch and annihilate in turbulence - annihilation is more subtle

Strong turbulence scenario:



Weak turbulence scenario:



Weak-turbulence ($u' << S$) analysis shows unexpectedly complicated dependences

- v is found to depend on the shape of the velocity power spectrum as well as on u'/S
- For strong turbulence, the analysis implies at least this degree of complexity
- Further progress faces formidable obstacles

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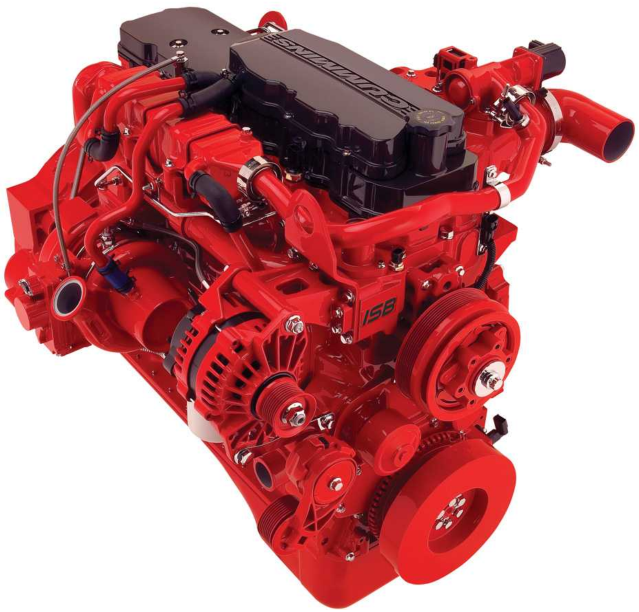
Cummins has, this year, marketed the first all-computationally-designed diesel engine

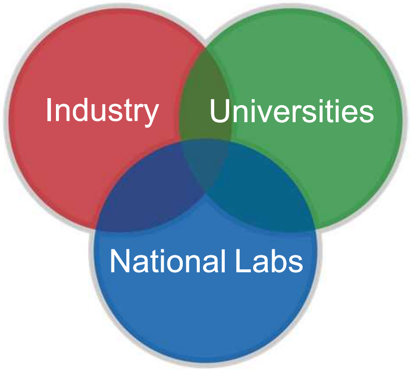


2007 ISB (6.7 liter diesel)

- In contrast with the traditional iterative build-and-test approach:
  - After-the-fact testing only
  - More robust design
    - larger parameter space explored
  - Improved fuel economy
  - Emission compliant (new 2007 regs)
  - Reduced development time and cost

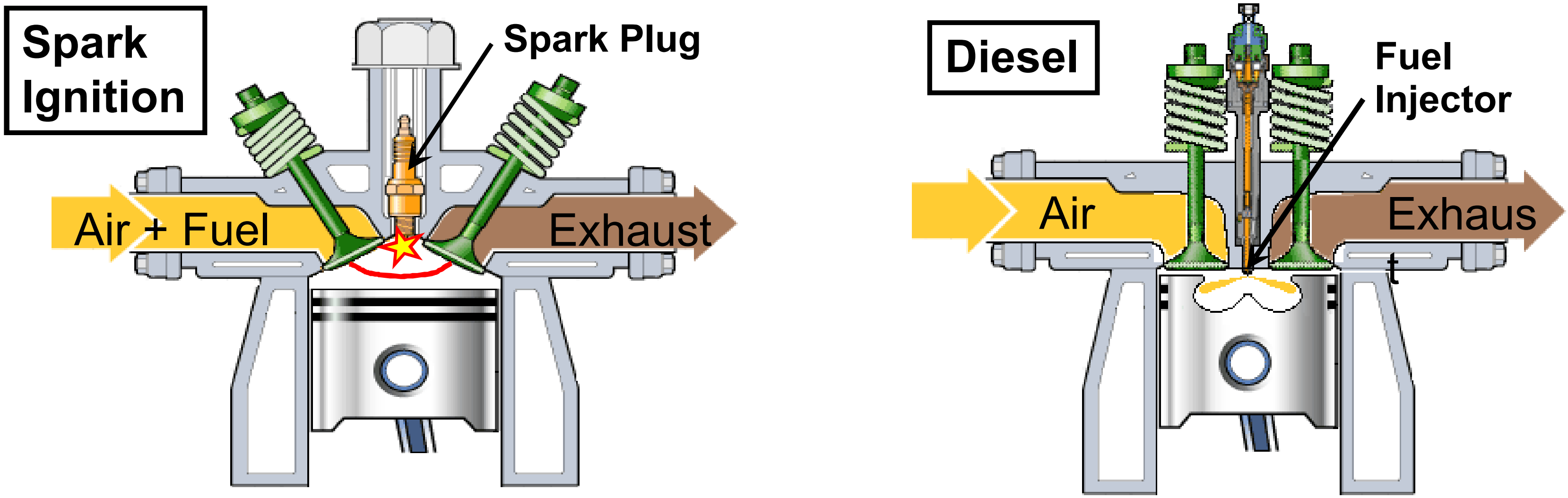
Achieving this milestone was a multi-institutional effort

- Resulted from a DOE–supported collaborative partnership between industry, national laboratories, and universities
- Sandia provided a key enabling component – new fundamental understanding of the physical and chemical processes controlling diesel combustion
- LLNL, LANL, and various universities developed models based on this physical understanding



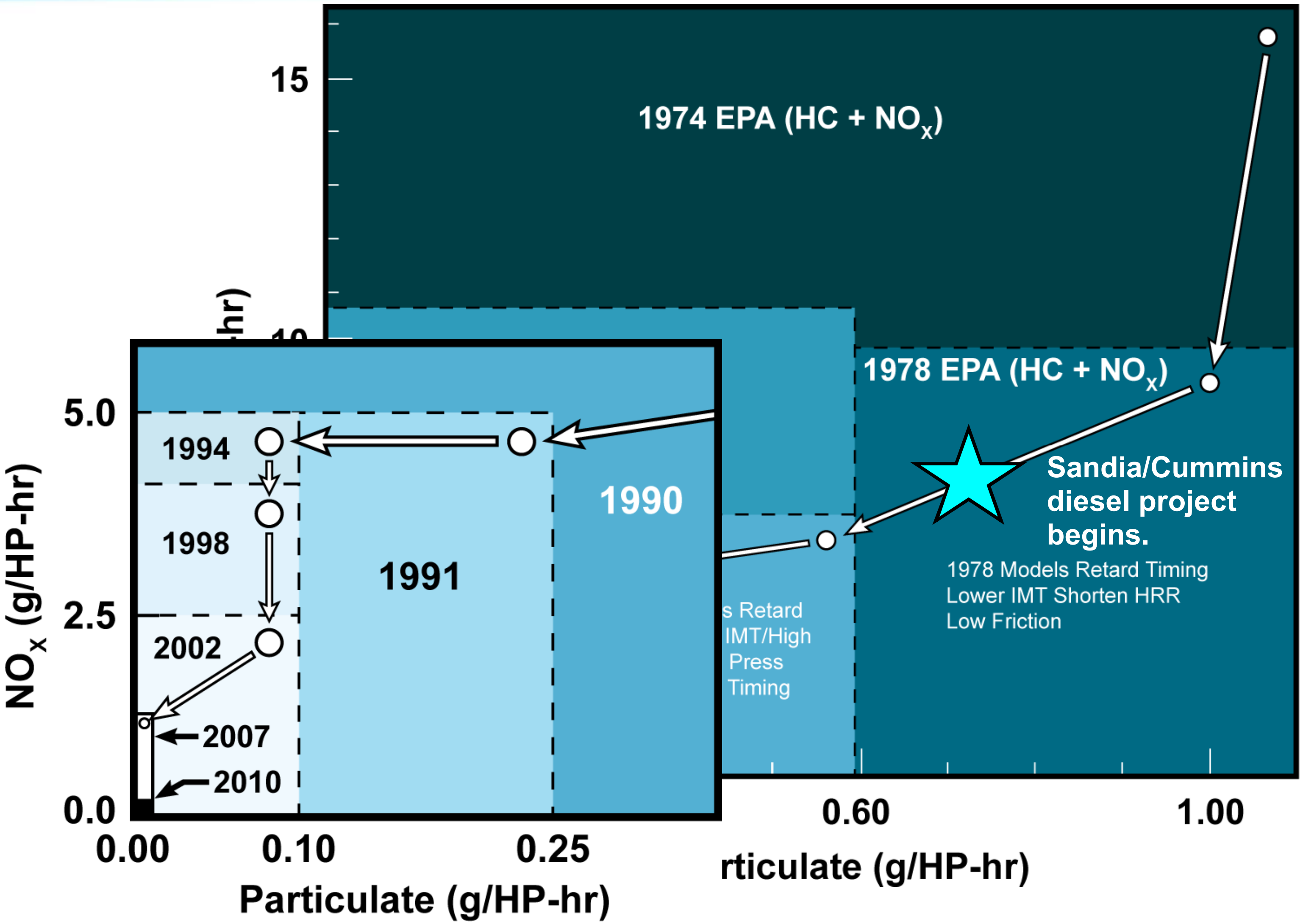
2007 ISB 6.7 liter diesel

How do diesel engines work?



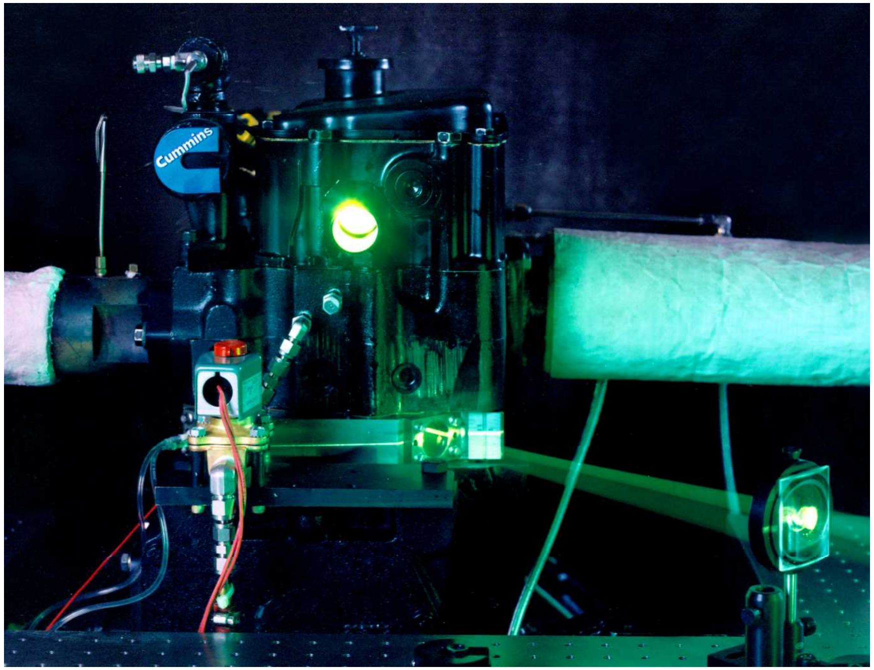
- In a diesel engine, fuel autoignites and burns as it is injected into compression-heated air
- Load is controlled by the amount of fuel injected
- High compression ratio and absence of throttle losses result in thermodynamic efficiencies 30 – 40% higher than spark engines
- Jet-mixing and combustion processes are complex

Tightening diesel emission regulations drive technology



In response, industry sought laboratory expertise

- In the late 1980’s Cummins asked Sandia to apply laser diagnostics to diesel combustion in a Cummins-supplied optical engine to provide the fundamental understanding (*science base*) needed to meet ever-more-stringent emission regulations
- The initial effort helped Cummins solve a soot-in-oil problem



Original diesel research engine had limited optical access.

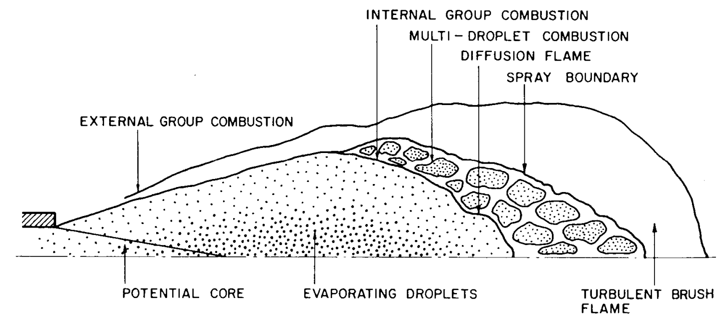
The effort broadened from problem solving to science-based understanding

- Key question – What really happens during diesel combustion?
  - When and where do soot and NO_X form?
  - How do fuel injection & air-mixing occur?

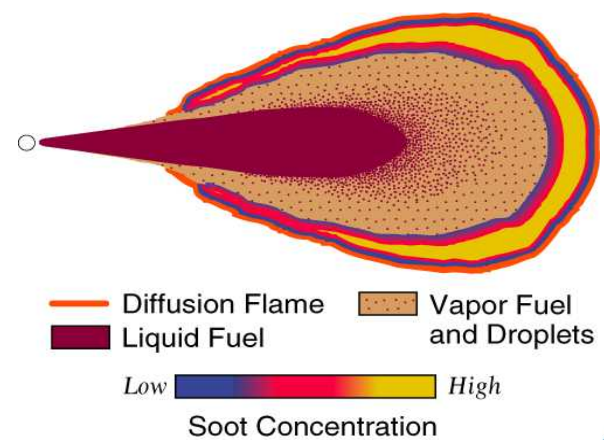
- It was generally thought that diesel combustion could be adequately described by steady-spray combustion theory (see the representative schematic)

- There was uncertainty about details
  - droplet combustion?
  - droplet-cluster combustion?
  - single diffusion flame envelope?

Old description of diesel combustion



Schematic of group combustion for a fuel spray.
From Kuo, as adapted from H. Chiu and Croke



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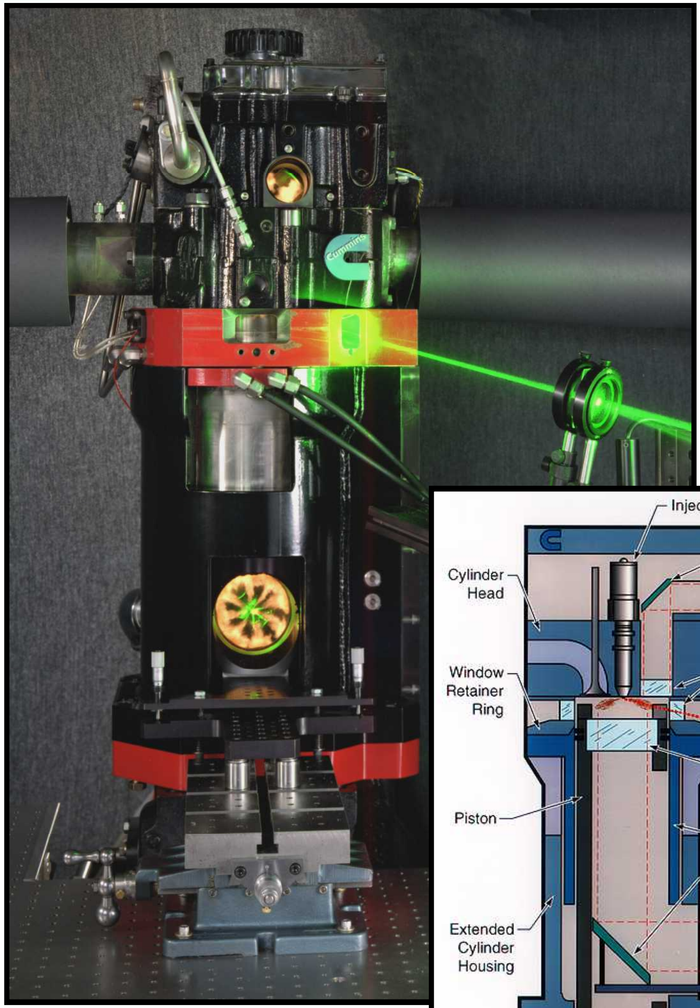
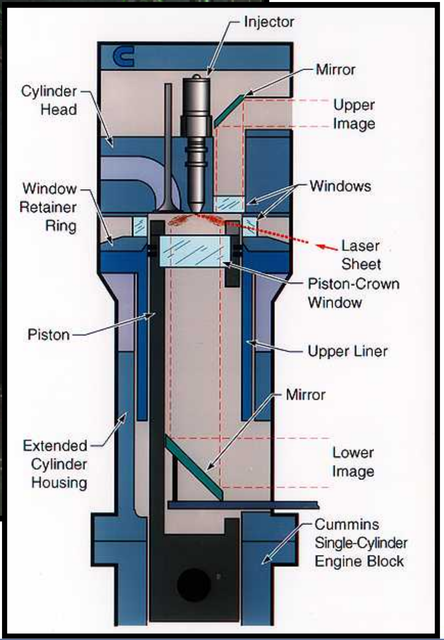
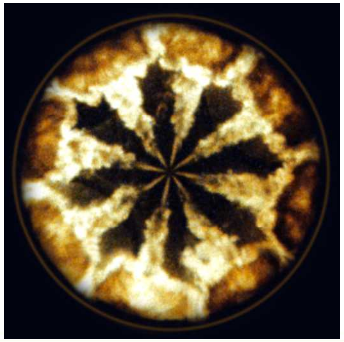
Sandia designed and built a heavy-duty diesel research engine





- Approach: Substantially increase optical access while maintaining the basic geometry and combustion characteristics of a production engine
- Investigate in-cylinder processes under realistic operating conditions
- Apply multiple advanced laser diagnostics to investigate all aspects of diesel combustion and emissions formation

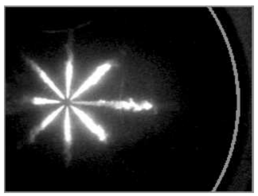


High-speed photo of Diesel combustion

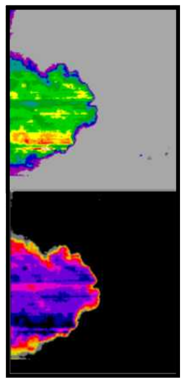
Laser-imaging diagnostics changed our understanding of diesel combustion

Numerous advanced diagnostics were applied during a decade of research

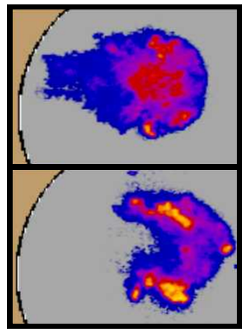
Liquid spray



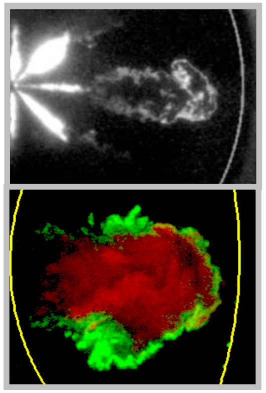
Mixture & Temp.



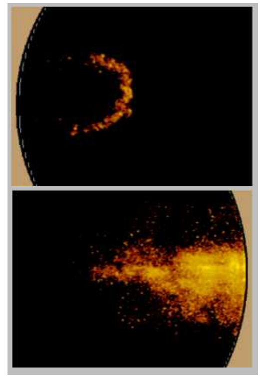
Soot: LII and Mie



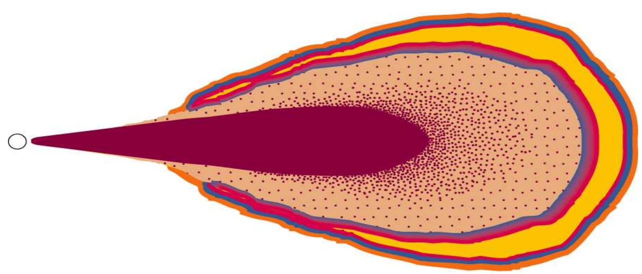
OH PLIF & LII



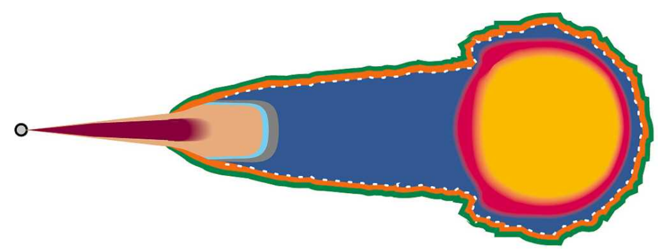
NO PLIF



Old Description



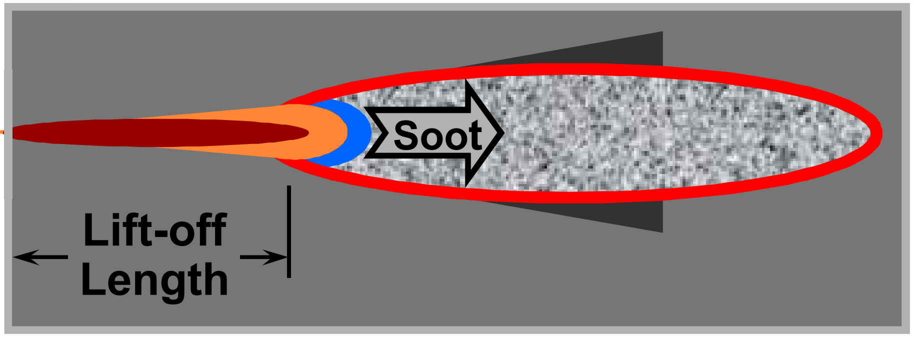
New Conceptual Model

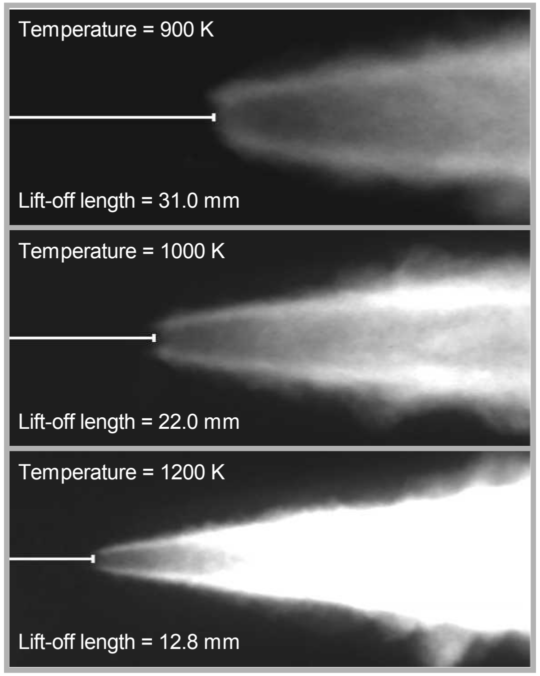


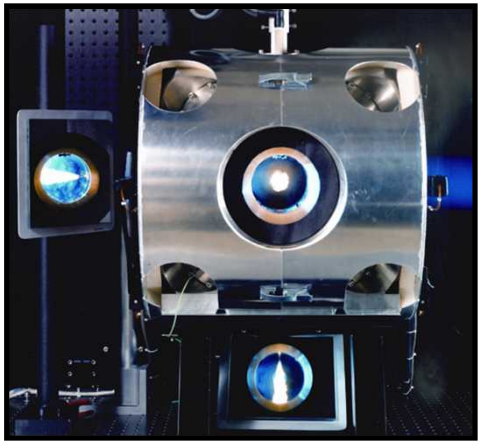
Results spurred new directions in diesel-combustion R&D, even before full model development

A diesel combustion simulation vessel was built to study jet mixing and flame lift-off

- Simulation vessel provided a unique capability to reach P, T, and injection parameters well beyond the range of current engines
- Flame lift-off varies significantly with operating conditions
- A scaling law for jet mixing developed that predicts jet parameters, including liquid length and fuel/air mixture at lift-off

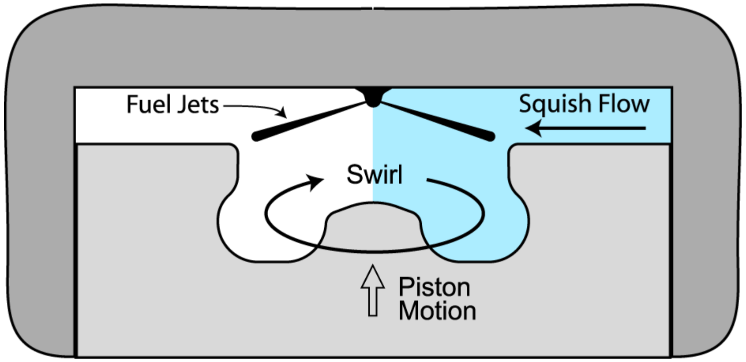


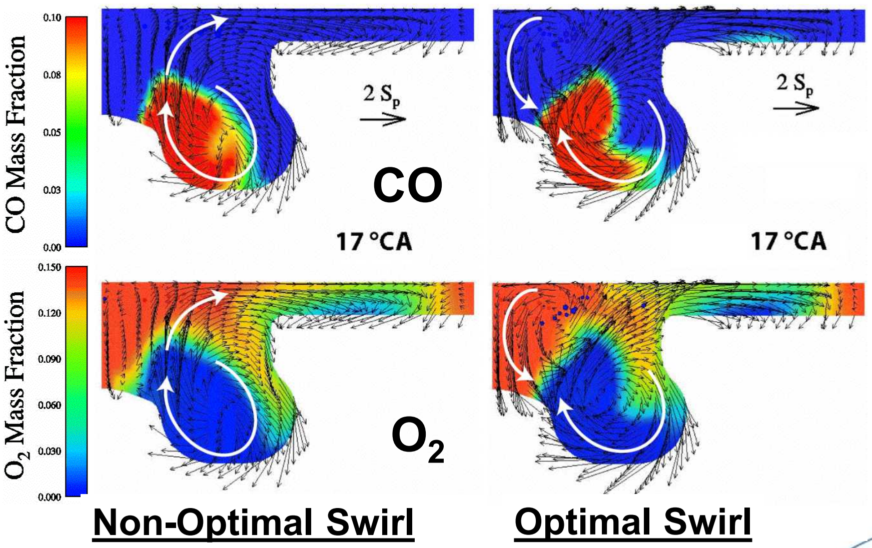




Secondary mixing can improve diesel combustion

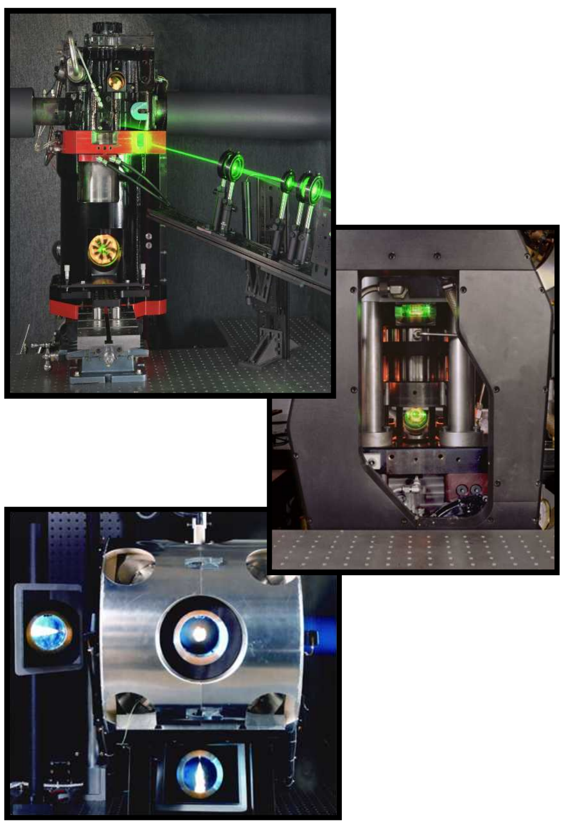
- Jet-mixing alone is often not sufficient, particularly for automotive-sized engines
- Bowl geometry and in-cylinder flows increase mixing and turbulence
- With a good design, jet/bowl interactions combine with swirl and squish flows to increase burn rate and soot burnout



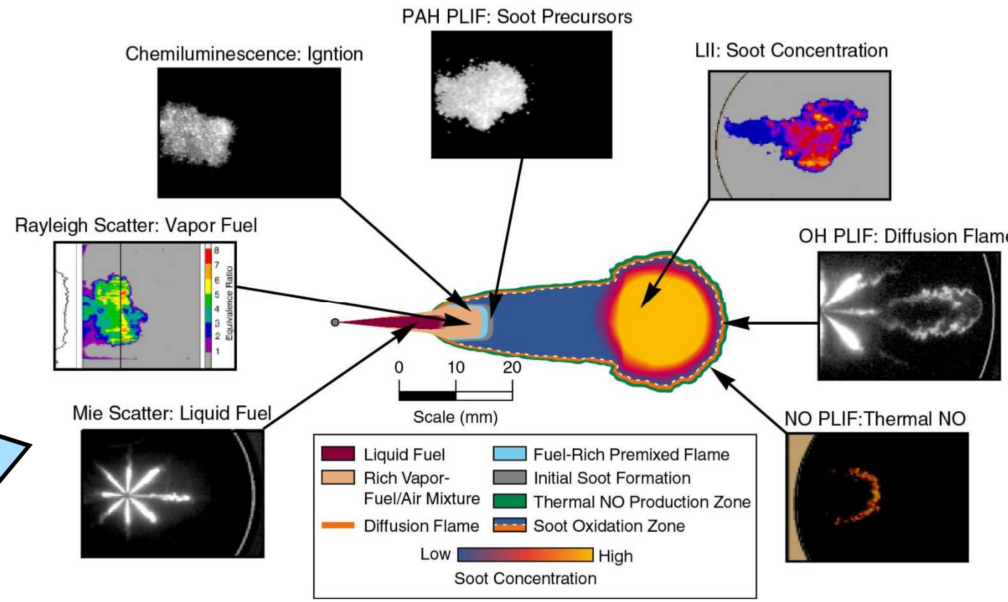


Combined results provide new physical understanding and enable science-based model development

Optical engines and laser diagnostics

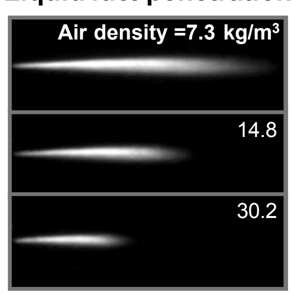


Diesel combustion

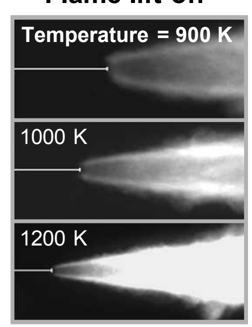


Scaling of critical processes

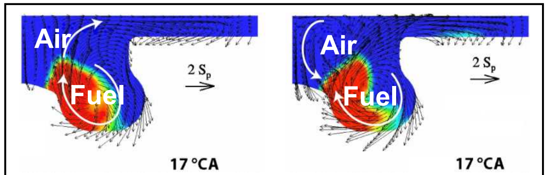
Liquid fuel penetration



Flame lift-off



In-cylinder flows



Non-optimal swirl **Optimal swirl**

As research progressed, the partnership grew

- Original partnership expanded to include multiple diesel and automotive companies in addition to Sandia, LLNL, and LANL
- It included close cooperation with DOE-funded university research

Partnerships carry research results to products

Based on the new physical understanding, the partners developed models of many aspects of diesel combustion

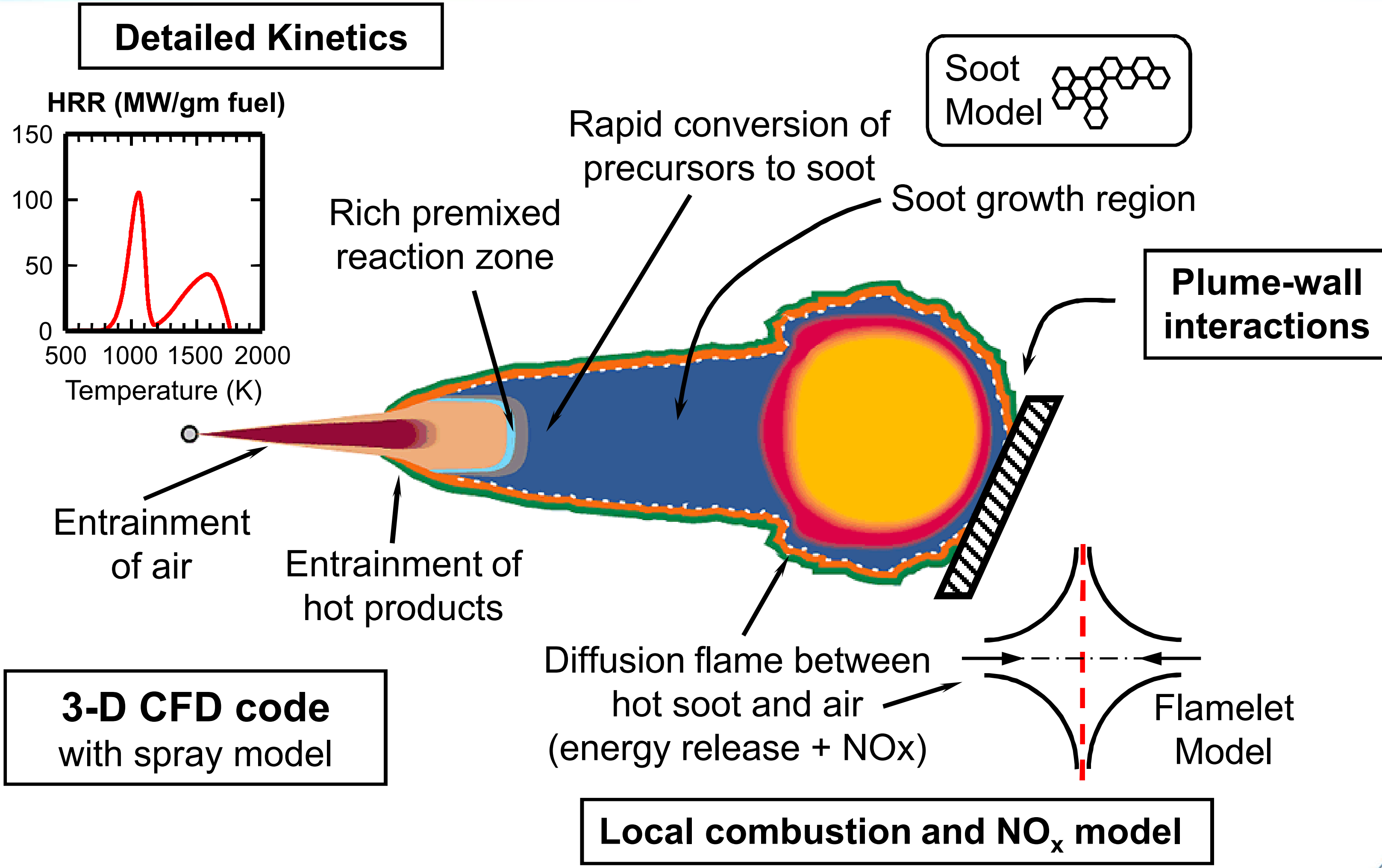


Figure from Cummins, Inc.

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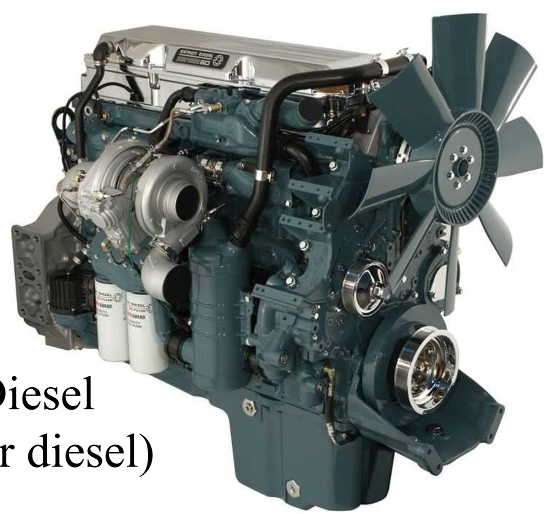
Industry has adapted and further developed these models into engine design tools

Cummins ISB
(6.7 liter diesel)

- All diesel makers now use science-based models derived from the DOE program for some parts of their design process
- Cummins is the first to announce a complete engine design using only computer modeling and analysis

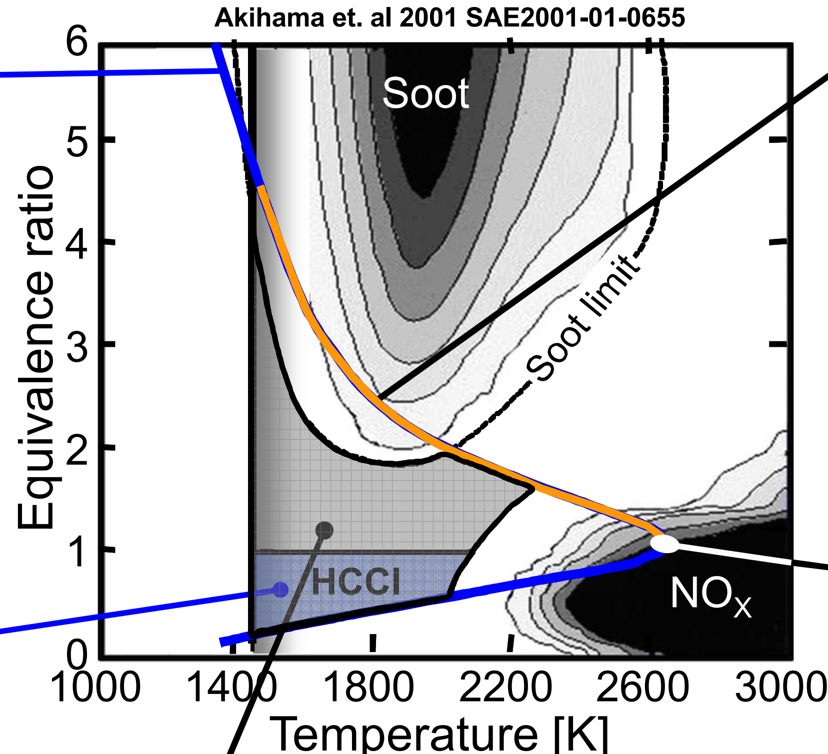


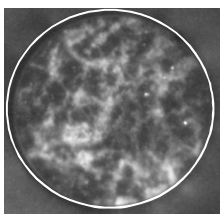
Detroit Diesel
(14.0 liter diesel)

Cat liter diesel)

Current Sandia research is focused on advanced combustion strategies that enable clean, high-efficiency engines

Adiabatic flame temperature in air





HCCI

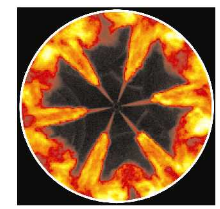
- A form of LTC that is mostly premixed
- Lean or diluted with exhaust gas

Low-Temperature Combustion (LTC)

- Diesel-like efficiency (high compression ratio and no throttling)
- Low NOx and particulate emissions
- Challenges: control of timing & HRR, and poor combustion efficiency at low loads

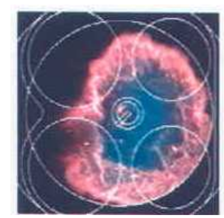
Diesel Combustion

- Controlled timing and heat-release rate (HRR)
- High efficiency (relative to spark ignition)
- NOx and PM emissions



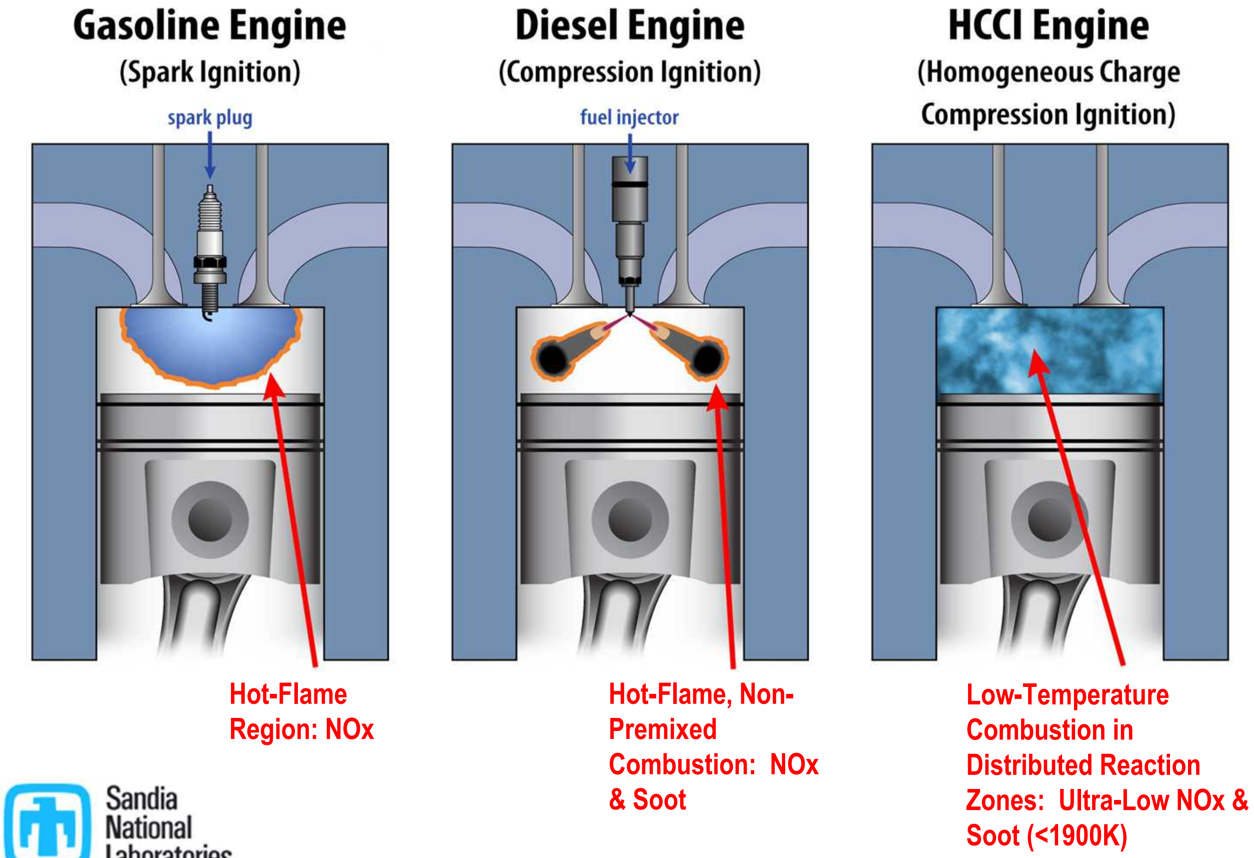
Spark-Ignition Combustion

- Controlled timing and HRR
- Three-way catalyst (low NOx)
- Low efficiency (relative to diesel)



How do HCCI and low-temperature combustion (LTC) Work?

- LTC includes HCCI and various other techniques in which diesel fuel is injected early and partially premixed prior to autoignition (PCCI)
- HCCI and other LTC schemes offer high efficiency & low emissions



- High Efficiency:
  - High compression ratio
  - No throttle
- Challenges:
  - Combustion phasing control
  - Low loads
  - High loads
  - Fuel-effects

The partnership continues to grow – five major energy companies recently joined

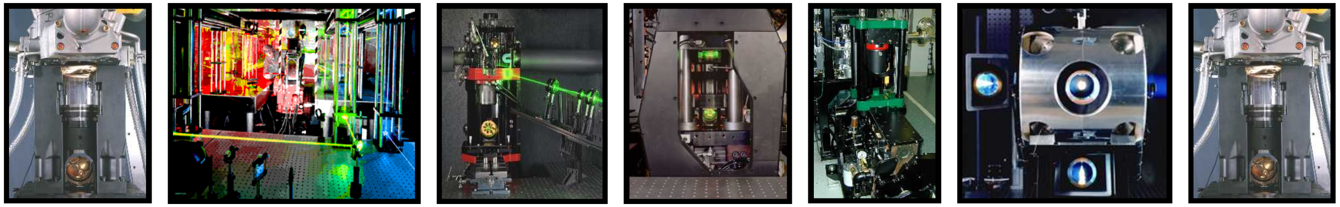
FreedomCAR & Fuel Partnership

21ST CENTURY TRUCK PARTNERSHIP

Ford
GM
Cummins
Mack DRIVEN
GE
ConocoPhillips
DAIMLERCHRYSLER
Chevron
Lawrence Livermore National Laboratory
CATERPILLAR
ExxonMobil
JOHN DEERE
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY
ARGONNE NATIONAL LABORATORY
DETROIT DIESEL
INTERNATIONAL
Shell Global Solutions
bp
Sandia National Laboratories
Los Alamos NATIONAL LABORATORY

Development of the science base for the next generation of engines and fuels continues

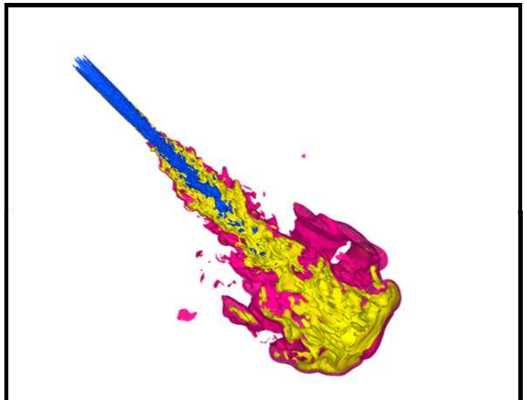
- Advanced low-temperature combustion strategies for enabling high-efficiency, low-emission engines (HCCI, PCCI, . . .).



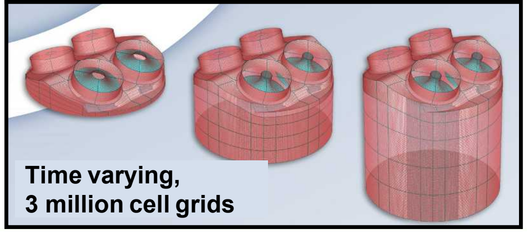
- Fuel effects are critical in these new-technology engines and future fuel sources will change.
  - bio-fuels ⇒ renewable
  - gas-to-liquid,
  - oil sand and shale
  - others . . .

Next generation computational tool:

large-eddy simulation (LES) of engines



LES jet simulation



Time varying,
3 million cell grids

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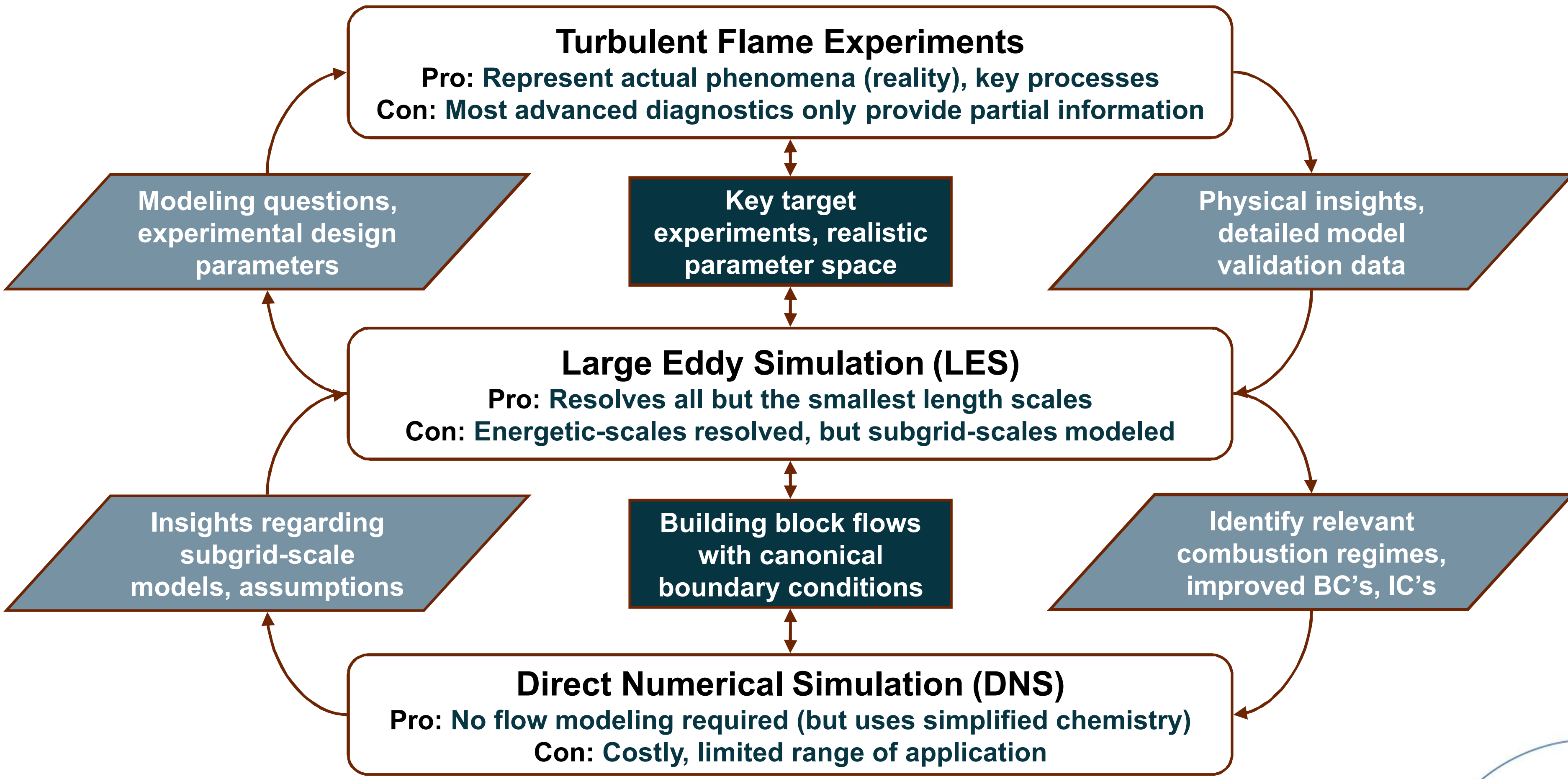
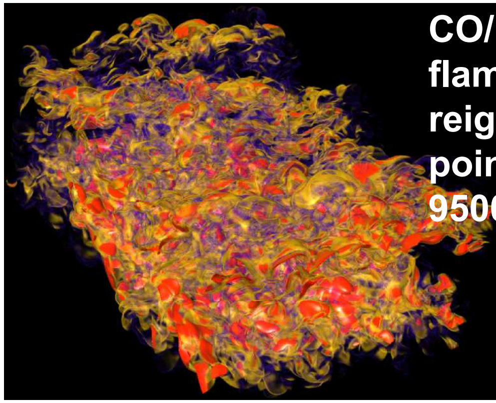
For engines and other applications, coordinated experimental and computational studies are the key to progress



DNS is a research tool and LES is moving toward application, but RANS is the main design tool

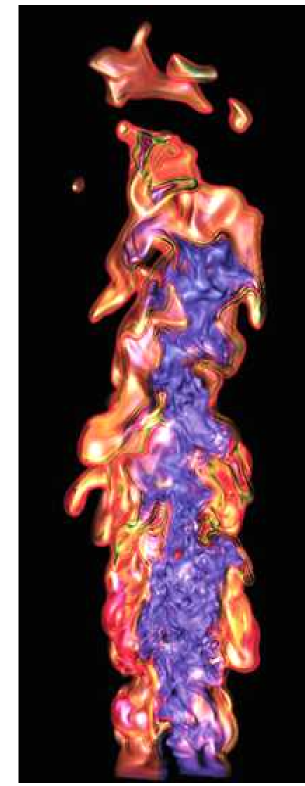
- Reynolds–Averaged Navier–Stokes (RANS)
  - Some unsteady applications, but mainly steady state
  - All but the largest flow scales are modeled empirically
  - Requires many tuning constants for calibration
- Large Eddy Simulation (LES)
  - Resolves all but the smallest scales
  - Unresolved scales are modeled
  - Dynamic modeling procedure reduces parameter tuning
- Direct Numerical Simulation (DNS)
  - No flow modeling required
  - Costly, limited range of application

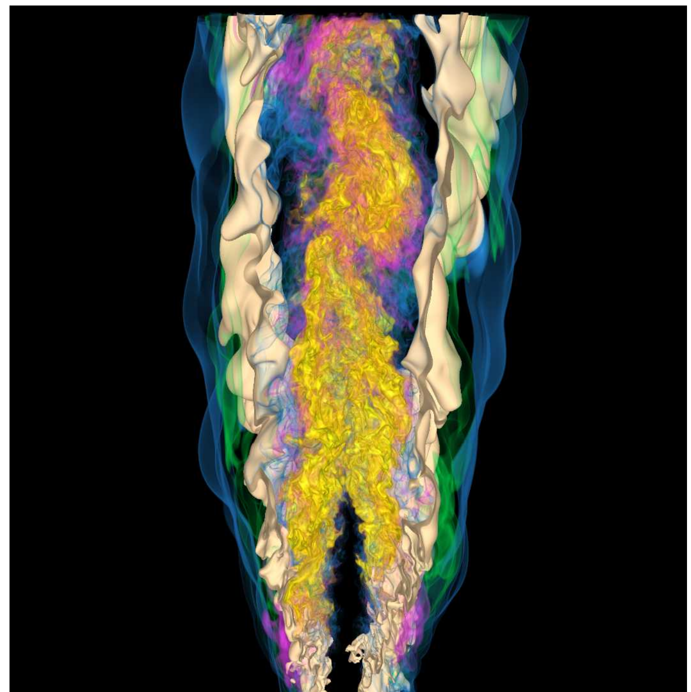
DNS is applied to canonical configurations to study small-scale combustion dynamics



CO/H_2 non-premixed flame, extinction & reignition, 500M grid points, Re_{slot} = 2500 to 9500

Lean premixed CH_4/Air flame, 200M grid points, Re_{slot} = 840, 1400, 2100, Re_t = 40, 75, 250

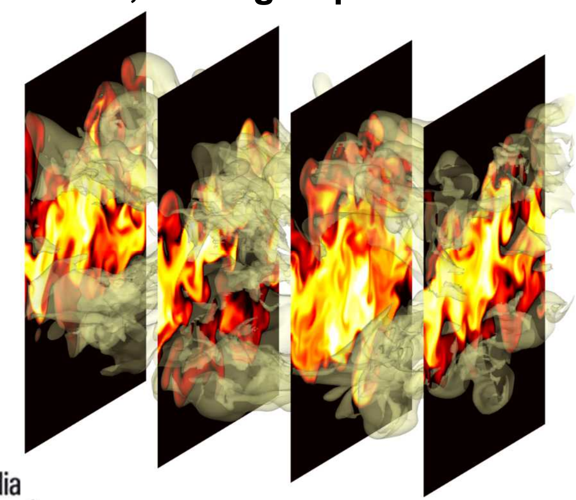




Lifted H_2/Air flame in vitiated coflow 1B grid points

Re_{slot} = 11000 Re_t = 400

Ethylene non-premixed sooting flame, 350M grid points



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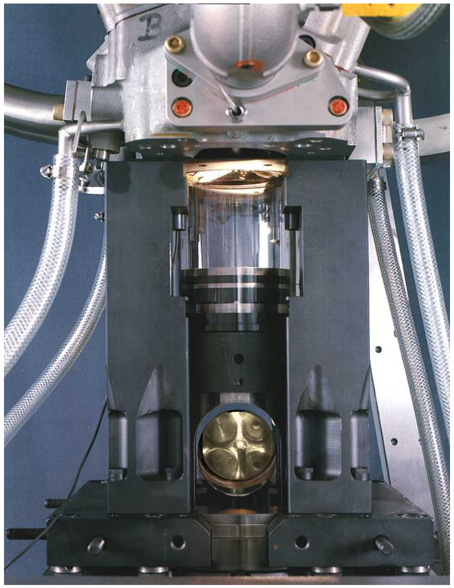
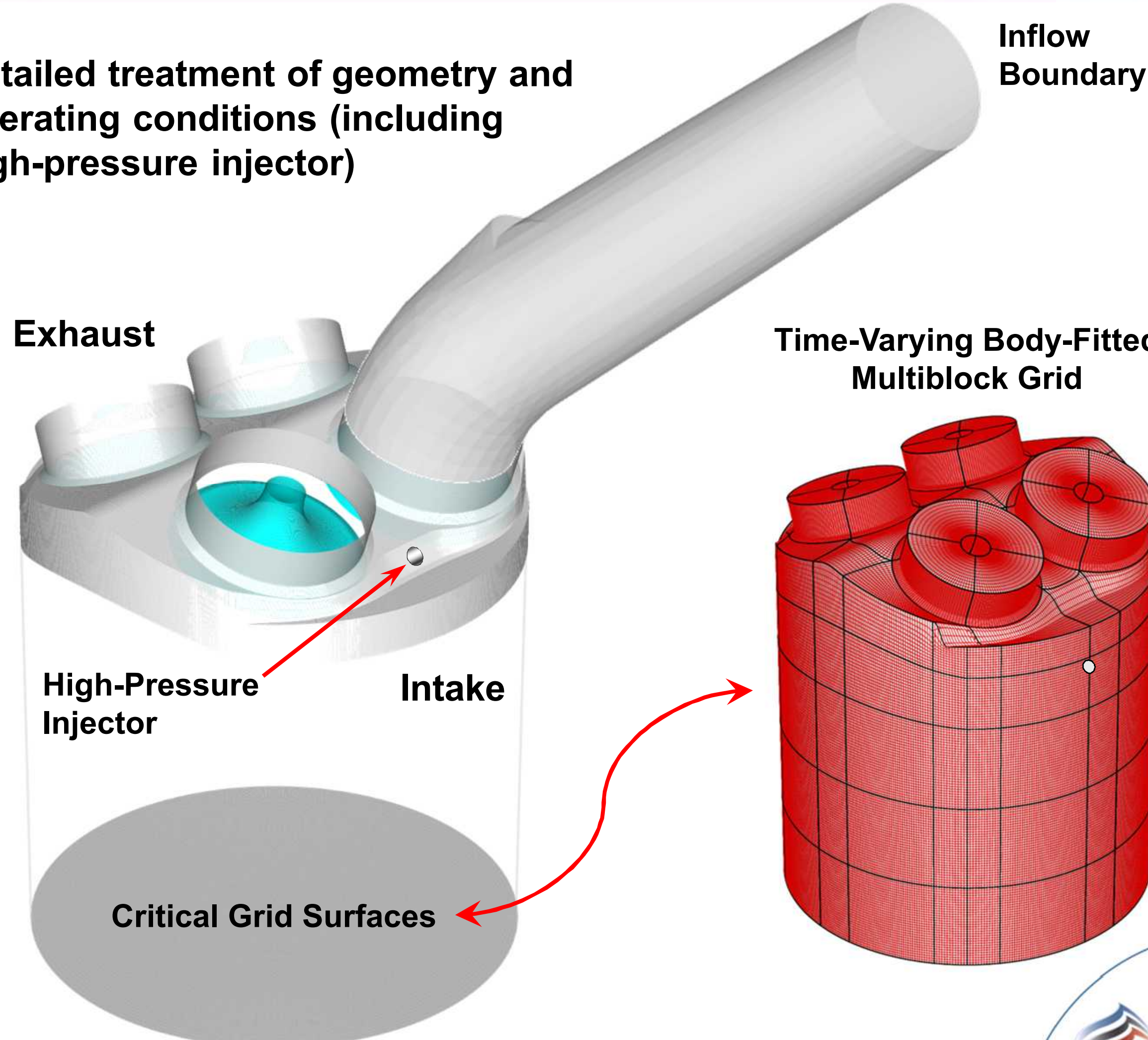
The size and operating conditions of internal combustion engines are suitable for LES application

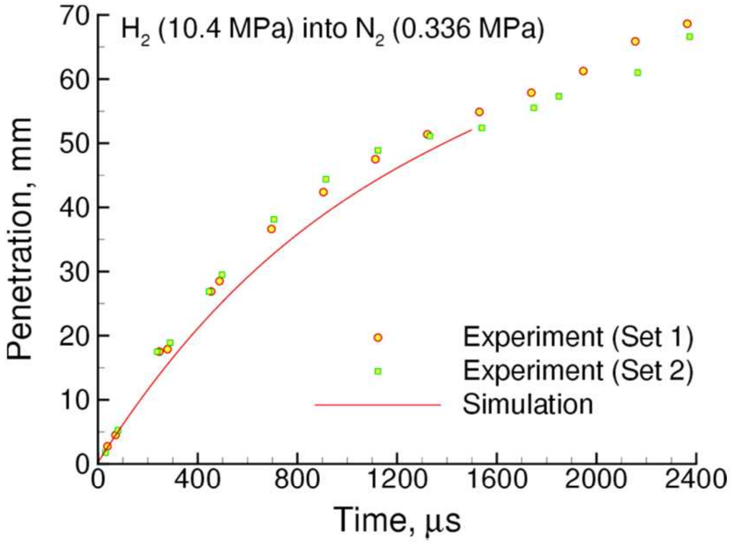


Engine Specifications	
Compression Ratio	9 – 12
Bore	92 *mm*
Stroke	85 *mm*
Peak Turbulence Intensity	2.85 *m/s*
Integral Length Scale	2 *mm*
Thermal Layer Thickness	6.3 *μm*
Kolmogorov Length Scale	5.6 *μm*
Reaction Zone Thickness	3.9 *μm*
Turbulent Reynolds Number	2550

Detailed treatment of geometry and operating conditions (including high-pressure injector)

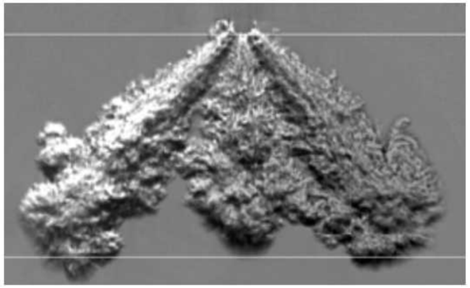


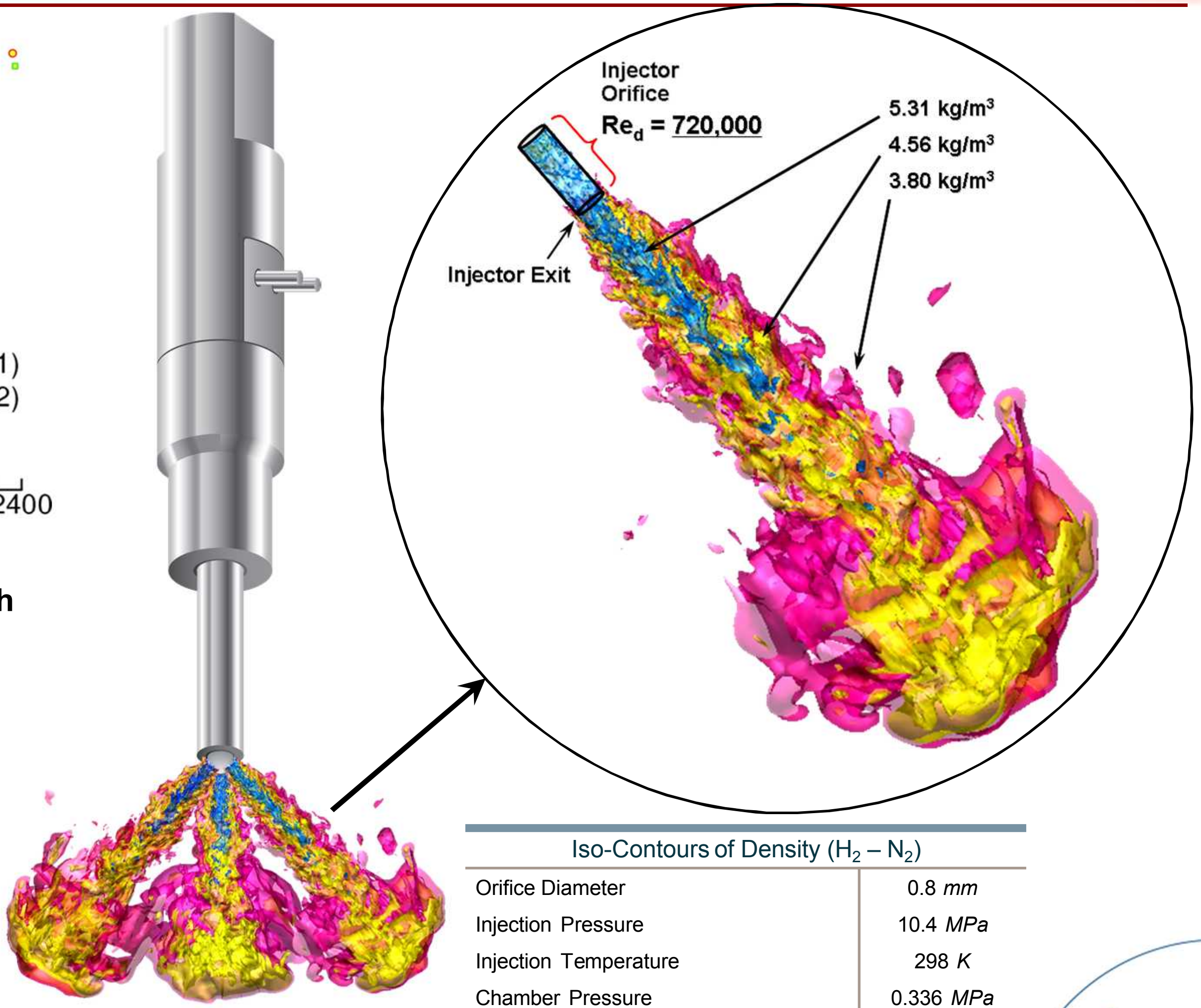
One focus of LES engine application is high-pressure injection



Representative comparison of LES with penetration measurements

Shadowgraph (U. Wisconsin)





Large Eddy Simulation

Iso-Contours of Density (H_2 – N_2)	
Orifice Diameter	0.8 *mm*
Injection Pressure	10.4 *MPa*
Injection Temperature	298 *K*
Chamber Pressure	0.336 *MPa*
Chamber Temperature	298 *K*

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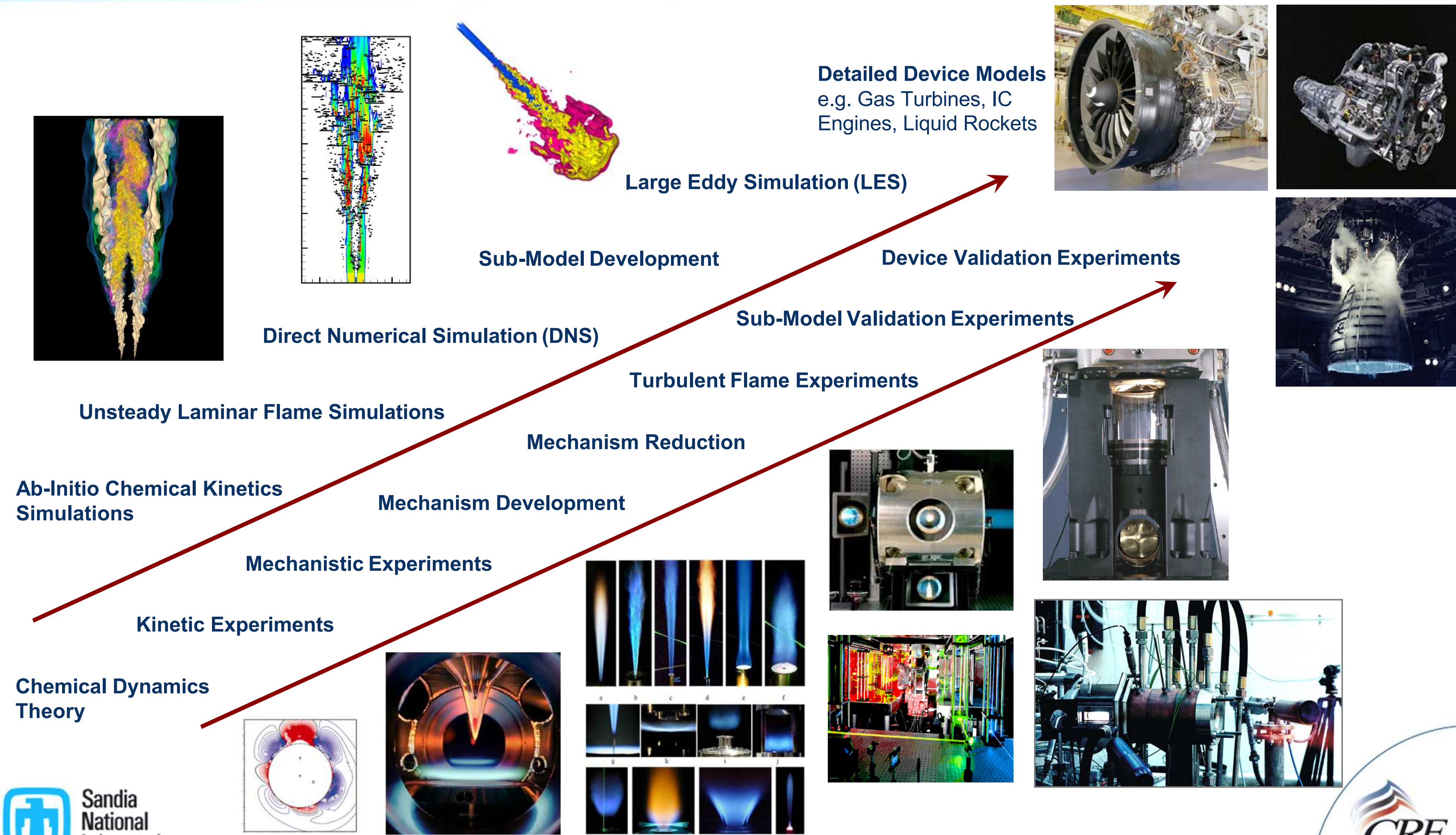
Science-based development of combustion technology involves a wide range of disciplines and tools



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Energy security and environmental sustainability deeply connect fuel research and combustion research

- New fuel feedstocks and oxidizer constituents ...
  - Biomass
  - Tar sands
  - Shale
  - Coal liquefaction
  - Hydrogen from electrolysis or hydrocarbon reforming
  - Pure oxygen instead of air (to enable carbon sequestration)
- will have wide-ranging combustion impacts such as
  - High flame temperature and radiation flux (hydrogen, pure oxygen)
  - High molecular diffusivity (hydrogen)
  - Modified ignition delay
  - Rheological effects on spray breakup and vaporization
- that broaden the range of combustion-related disciplines
  - Biosciences
  - …

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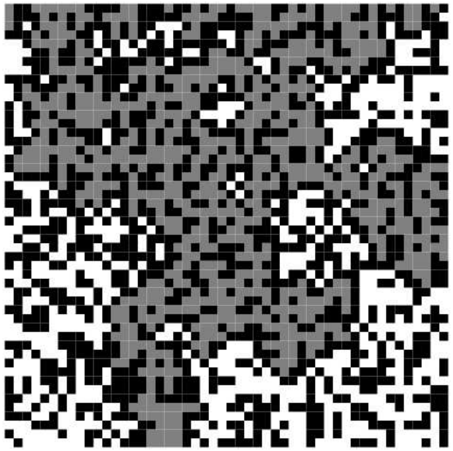
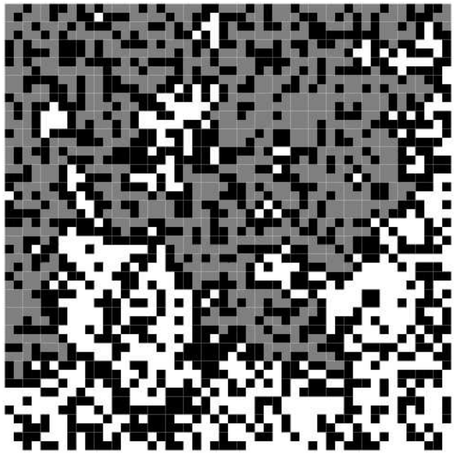
Percolation is a concept with broad applications in math, science, and engineering

- Example: 2D medium consists of squares, each of which is randomly assigned to be nonflammable (black) or flammable (gray or white)
- If the flammable fraction exceeds the 'percolation threshold,' then a flame ignited along the top edge propagates indefinitely (top), otherwise burning ceases (bottom)
- In an advecting (e.g., turbulent) medium, products and flammable reactants can be brought into contact, sustaining flame propagation in the absence of an infinite connected flammable region





Top-to-bottom percolation:

Gray region is reachable

No connected path to white region

Applications include spray combustion and lifted turbulent jet flames

As char particles oxidize, geometrically disconnected fragments are released

- Prior assumption: Mechanical attrition causes fragmentation
- Percolation mechanism implies fixed porosity at receding perimeter
- MIT group found experimental support for this mechanism
- Technology impact: more rapid char burnout in coal furnaces

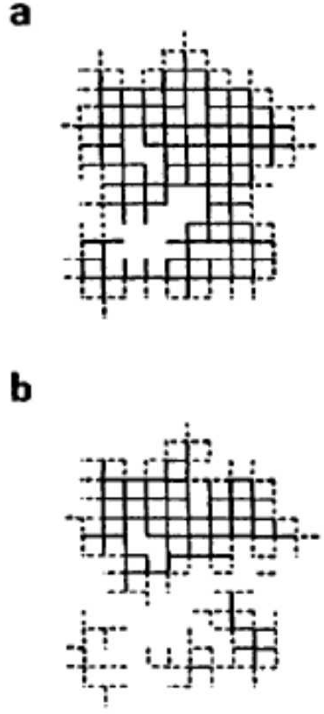
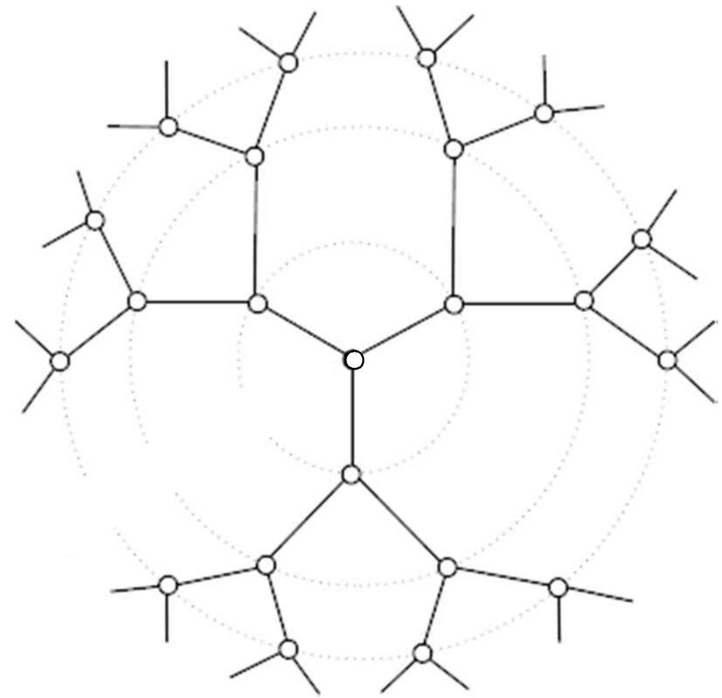


Fig. 1. Snapshots during the simulated burnout of a two-dimensional cluster. Unbroken (broken) line segments are unignited (ignited) solid bonds. (a) Initial cluster. (b) Configuration after partial burnout, exhibiting four fragments.

Idealizing the coal macromolecule as a tree enables percolation modeling of pyrolysis

- Each infinite branch is attached to the macromolecule
- For coordination number N, at least N bond cuts are needed to form a fragment (N=3 in sketch)
- The ‘chemical percolation devolatilization model’ uses NMR and reactor data to assign model parameters for prediction of product yields



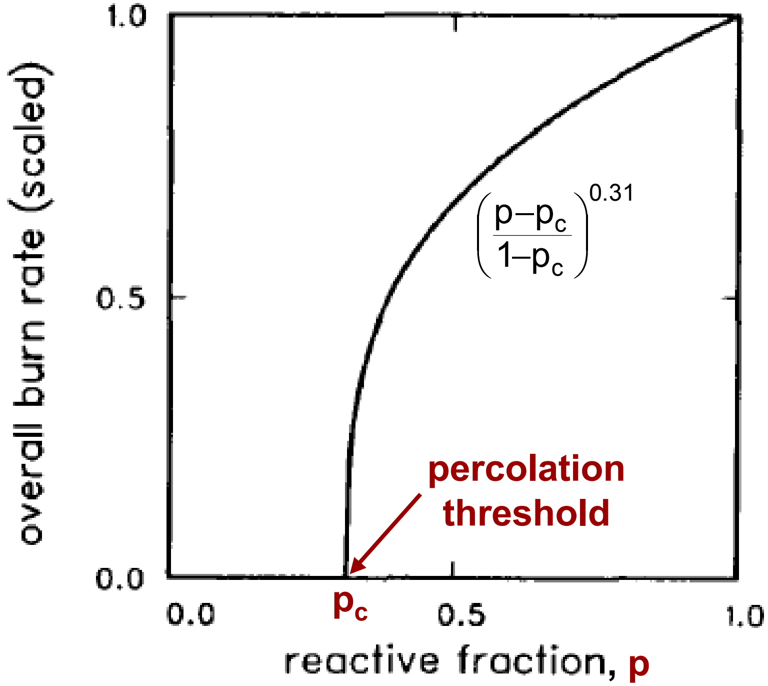
Bethe lattice: closed-form fragment-size distributions are known for any N and fraction p of uncut bonds

Combustion of a heterogeneous solid propellant can be idealized as a percolation problem

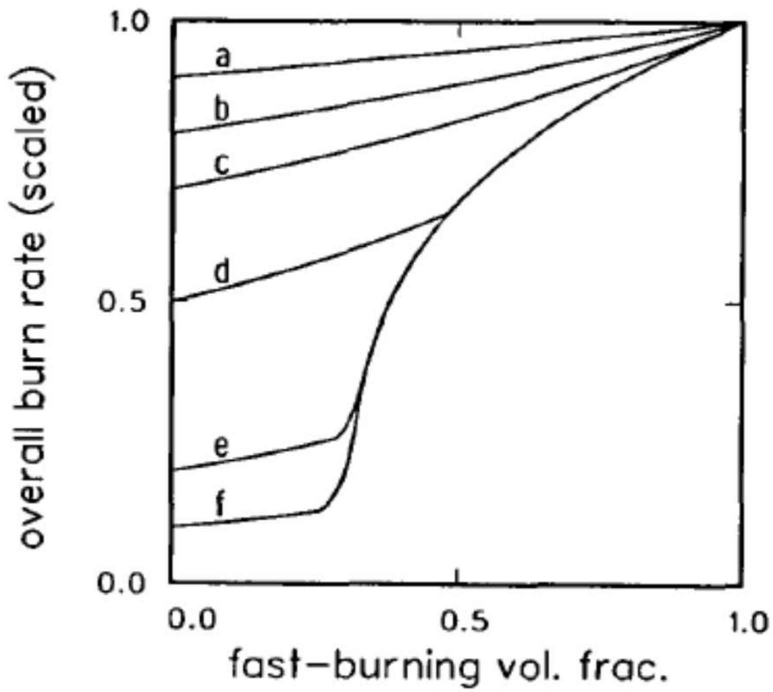
- N components, each with a different burn rate S
- What is the overall burn rate as a function of component volume fractions and burn rates?
- This is related to percolation because small amounts of slow-burning components can be bypassed, so their burn rates become irrelevant (they ultimately burn as particles in the product gas)

Known scaling behavior near the percolation threshold has been extrapolated heuristically

Two components,
one with nonzero S



Two components,
both with nonzero S



A variational method approximates a multi-component medium as a two-component 'effective medium' (Kerstein, 1987)

The model correlates the burn rates of 29 multi-component propellants using 4 free parameters

Propellant Designation	Relative wt% of Nominal AP Size Fraction (μm)								Burn Rate at Pressure (MPa)		
	400	200	90	50	20	6	2	0.7	3.45	6.89	13.8
SD III-2	—	—	36.15	—	15.66	—	—	48.19	1.53	2.95	5.61
SD III-3	—	—	—	—	63.85	—	—	36.15	2.34	3.68	5.82
SD III-4	—	36.15	—	—	27.70	—	—	36.15	1.61	2.97	4.85
SD III-5	48.19	—	—	—	15.66	—	—	36.15	1.20	2.21	4.32
SD III-6	—	—	—	36.15	15.66	36.15	12.04	—	1.87	2.95	4.42
SD III-8	—	—	—	36.15	27.70	—	36.15	—	1.73	2.79	4.50
SD III-9	—	36.15	—	—	27.70	—	36.15	—	1.60	2.77	4.62
SD III-10	48.19	—	—	—	15.66	—	36.15	—	1.27	2.29	4.06
SD III-12	—	—	36.15	—	15.66	48.19	—	—	1.72	2.62	4.04
SD III-14	—	36.15	—	—	27.70	36.15	—	—	1.62	2.48	3.79
SD III-15	48.19	—	—	—	15.66	36.15	—	—	1.14	1.79	2.97
SD III-16	—	36.15	—	36.15	27.70	—	—	—	1.03	1.43	1.93
SD III-17	—	—	36.15	—	63.85	—	—	—	1.53	2.12	2.95
SD III-18	—	—	48.19	—	51.81	—	—	—	1.32	1.82	2.43
SD III-19	—	36.15	—	—	63.85	—	—	—	1.36	1.99	2.85
SD III-20	48.19	—	—	—	51.81	—	—	—	.935	1.37	2.17
SD III-21	36.15	36.15	—	12.04	15.66	—	—	—	.610	.838	1.11
SD III-22	36.15	—	—	48.19	15.66	—	—	—	.953	1.33	1.80
SD III-23	—	48.19	—	36.15	15.66	—	—	—	.843	1.19	1.60
SD III-24	—	36.15	—	48.19	15.66	—	—	—	.998	1.36	1.86
SD III-25	48.19	—	—	36.15	15.66	—	—	—	.772	1.13	1.66
SD III-26	—	—	53.20	—	46.80	—	—	—	1.20	1.63	2.12
SD III-27	59.00	—	—	—	25.00	—	16.00	—	.678	.975	1.66
SD III-28	54.50	—	—	13.00	32.50	—	—	—	.701	.978	1.58
SD III-29	50.00	—	36.00	—	—	14.00	—	—	.704	.942	1.22
SD III-30	—	37.88	—	—	62.12	—	—	—	1.21	1.71	2.54
SD III-31	59.00	—	—	—	8.95	—	32.05	—	.653	.930	1.58
SD III-32	48.19	—	—	—	33.49	—	18.32	—	.947	1.58	2.44
SD III-33	48.19	—	—	—	42.65	—	9.16	—	—	1.47	—

The multi-component model has 1 free parameter p_c
(the others relate particle size to particle burn rate)

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