Challenges in Combustion

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GCEP Research Symposium
Meeting the Challenge of Reducing Global GHG Emissions Through Energy Research

June 13-16, 2005

Background: Greenhouse Emissions are Driven by Combustion and Transportation.

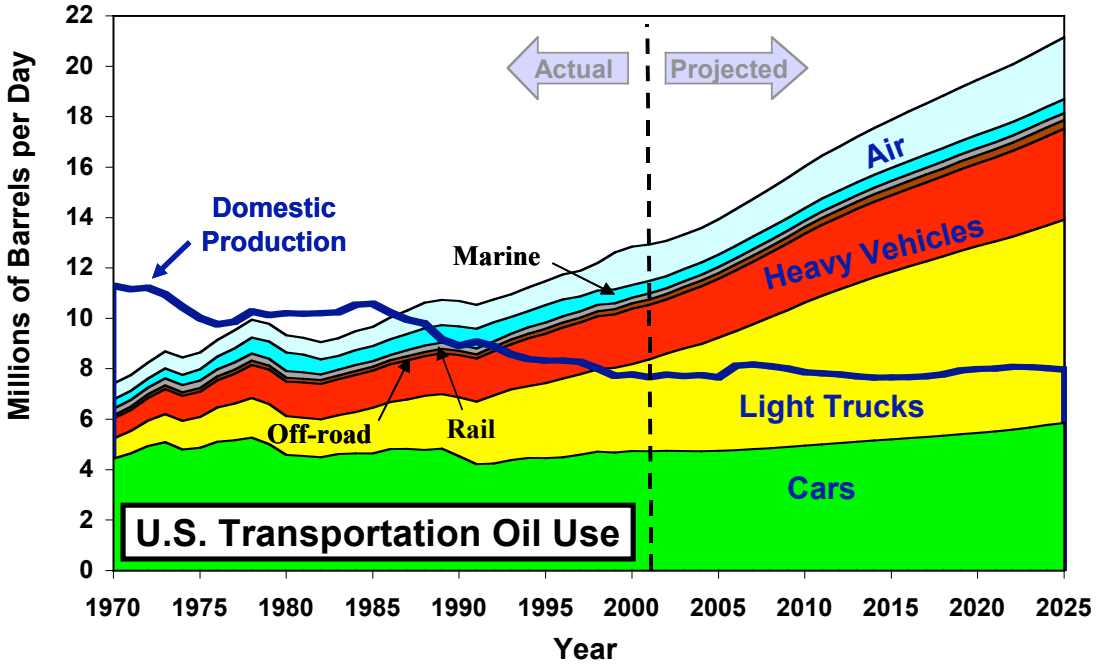
- Combustion accounts for 85% of all current power production in the United States
- Transportation accounts for 2/3 of our oil consumption.
  - Transportation consumption expected to increase 60% by 2025.

- Transportation is a major contributor to greenhouse gases.

Highway Carbon Emissions

(million metric tons)

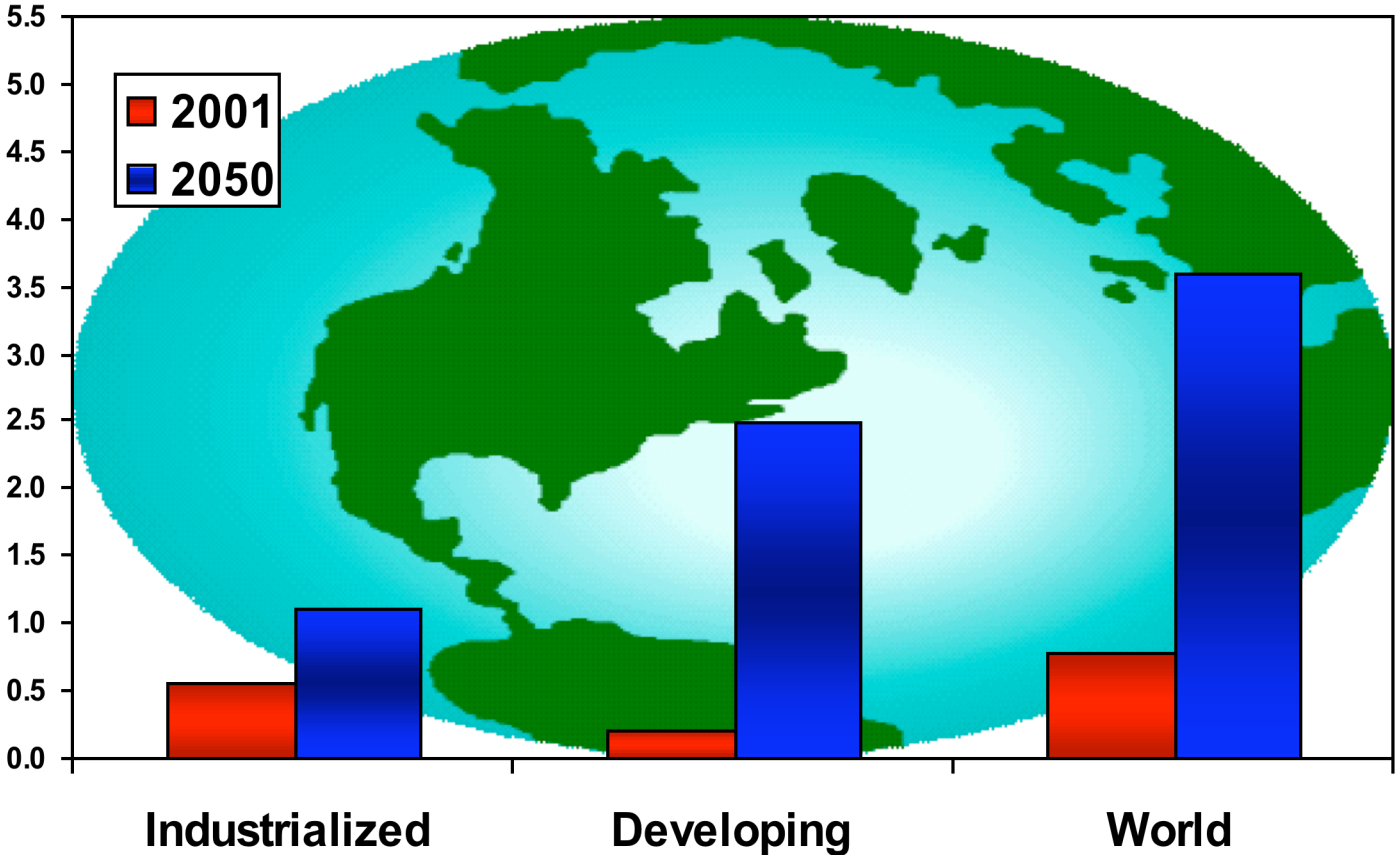
1990	2000	2010	2020
325	381	489	592



Source: Transportation Energy Data Book: Edition 22, September 2002, and EIA Annual Energy Outlook 2003, January 2003

Global Demand for Transportation is Expected to Increase Dramatically.

- Large increase in vehicle usage will increase demand for fuel.
- Increased carbon emissions - greenhouse gases.



These Facts Place Serious Challenges on the Transportation Industry.

- Engine manufacturers must simultaneously reduce:
  - Fuel Consumption
  - Carbon Emissions

  } Improved Engine Efficiency
  - Toxic Emissions: NO_X, Particulates (PM), Hydrocarbons (HC), & CO.
- The demand for these improvements is worldwide.
- American diesel engine companies are major exporters.
  - Important contribution to American jobs and balance of trade.
- American automotive companies have worldwide operations.
  - Important for the overall strength of these companies.
- Strong international competition to build clean and efficient engines.
  - American companies must be competitive in this global market.

Combustion research was alive and well in the 1600's.

FUMIFUGIUM:

OR,

The Inconvenience of the AER,

AND

SMOAKE of LONDON

DISSIPATED.

TOGETHER

With ſome REMEDIES humbly propoſed

By J. E. Eſq;

To His Sacred MAJESTIE,

AND

To the PARLIAMENT now Aſſembled.

Publiſhed by His Majeſties Command.

Lucret. l. 5.

Carbonumque gravis vis, atque odor inſinuatur
Quam facile in cerebrum?——

LONDON:

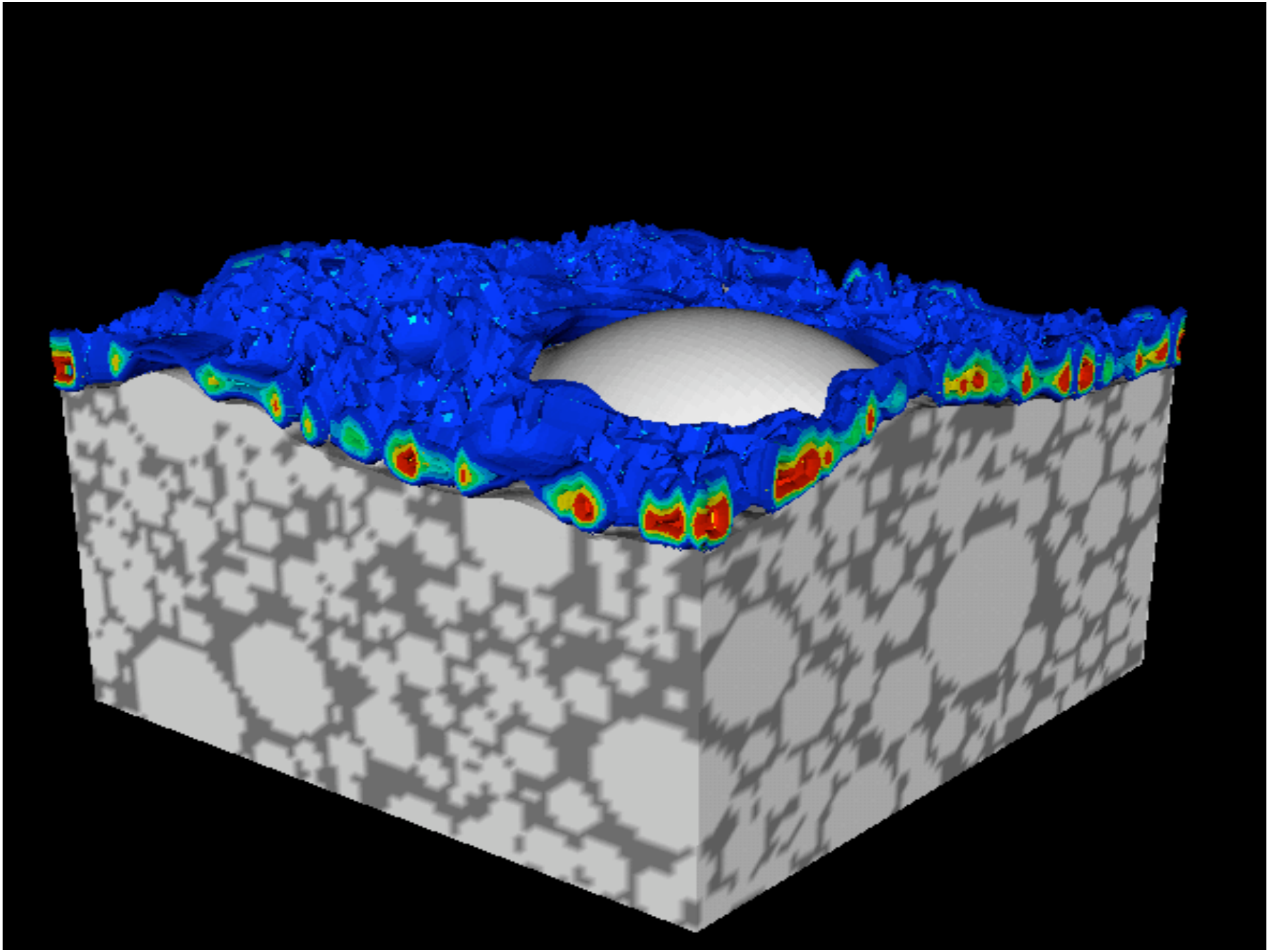
Printed by W. GODBID, for GABRIEL BEDEL, and THOMAS COLLINS; and are to be ſold at their Shop at the Middle Temple Gate, neer Temple Bar. M.DC.LXI.

Re-printed for B. WHITE, at Horace's Head, in Fleet-ſtreet. MDCCLXXII.

FIG. 1. Fumifugium by John Evelyn, London, 1661.

Combustion science is evolving steadily

- Computer simulation is becoming much more important
- Multiphysics submodels built into a 3D CFD framework is becoming common
- Massively parallel computing is having a big impact
- Many opportunities for “full system” simulations and direct comparisons with actual device experiments
- Corresponding need for greater fidelity in these submodels



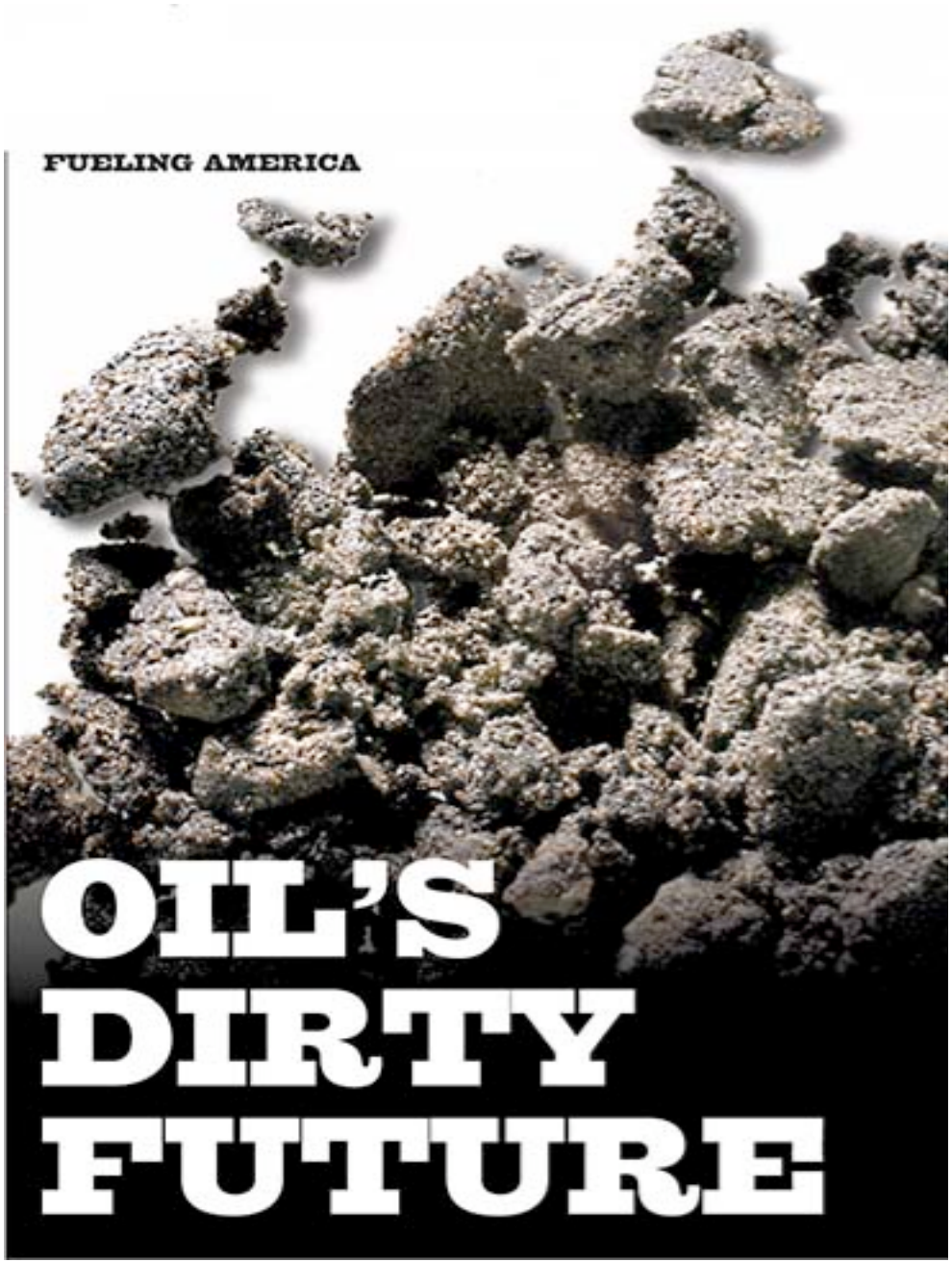
The dilemma of Canada's oil sands

JOE SHOULAK / *The Chronicle*

Canadian oil sands

- Second only to Saudi Arabia in proven oil reserves
  - Saudi Arabia 262 billion barrels
  - Canada oil sands 175 billion barrels
  - Arctic National Wildlife Refuge 10 billion barrels (est)
- Currently largely strip mined
- Even production is a serious source of greenhouse gases
  - 2 tons of sand produce one barrel of oil
  - production of one barrel of oil = daily emissions from 4 cars
  - huge usage of natural gas for extraction

Articles and pictures from SF Chronicle May 22-23



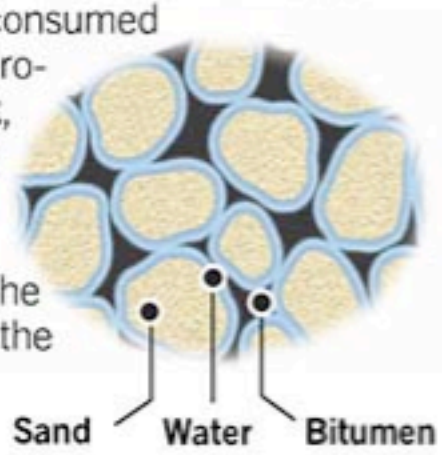
Athabasca oil sands

Chronicle / Brant Ward

Strip mining oil sands, using 400 ton capacity trucks

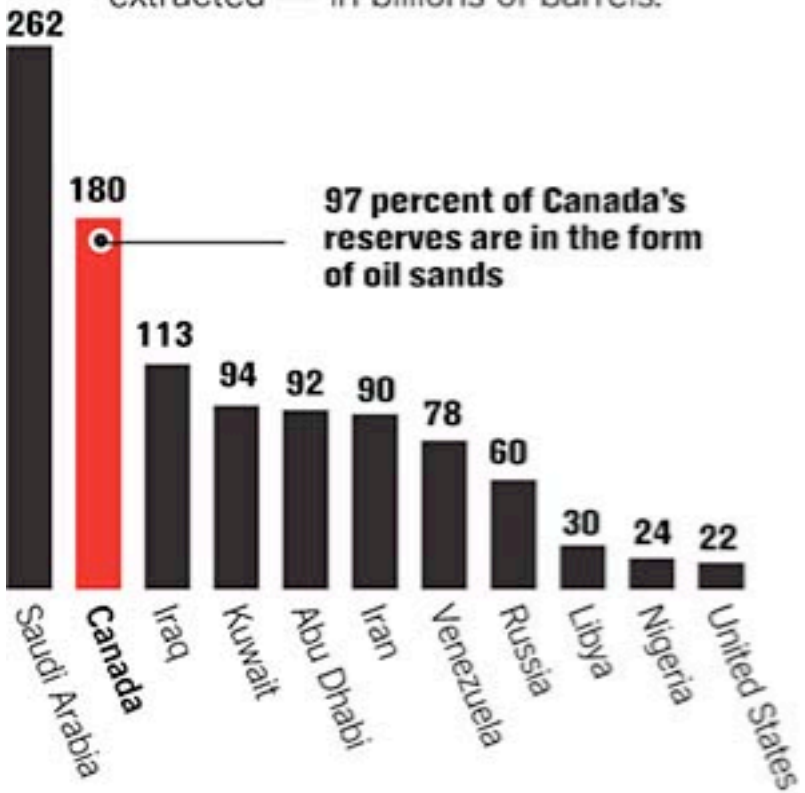
WHAT ARE OIL SANDS?

Fifty-million years ago, huge deposits of oil were pushed up through the Earth in what is now Canada. Bacteria consumed much of the lighter hydrocarbons, leaving a thick, sticky mixture of heavy petroleum called bitumen mixed with water and sandstone. The deposits cover an area the size of Florida.



GLOBAL CRUDE OIL RESERVES

Estimates of "proven" oil reserves — known existing deposits that can be profitably extracted — in billions of barrels.



Source: Suncor Energy Inc., Petroleum Communication Foundation, Oil and Gas Journal

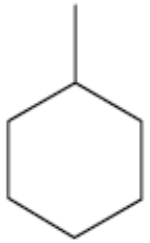
The Denver Post

DOE recently hosted a conference to assess current knowledge about transportation uses of these fuels

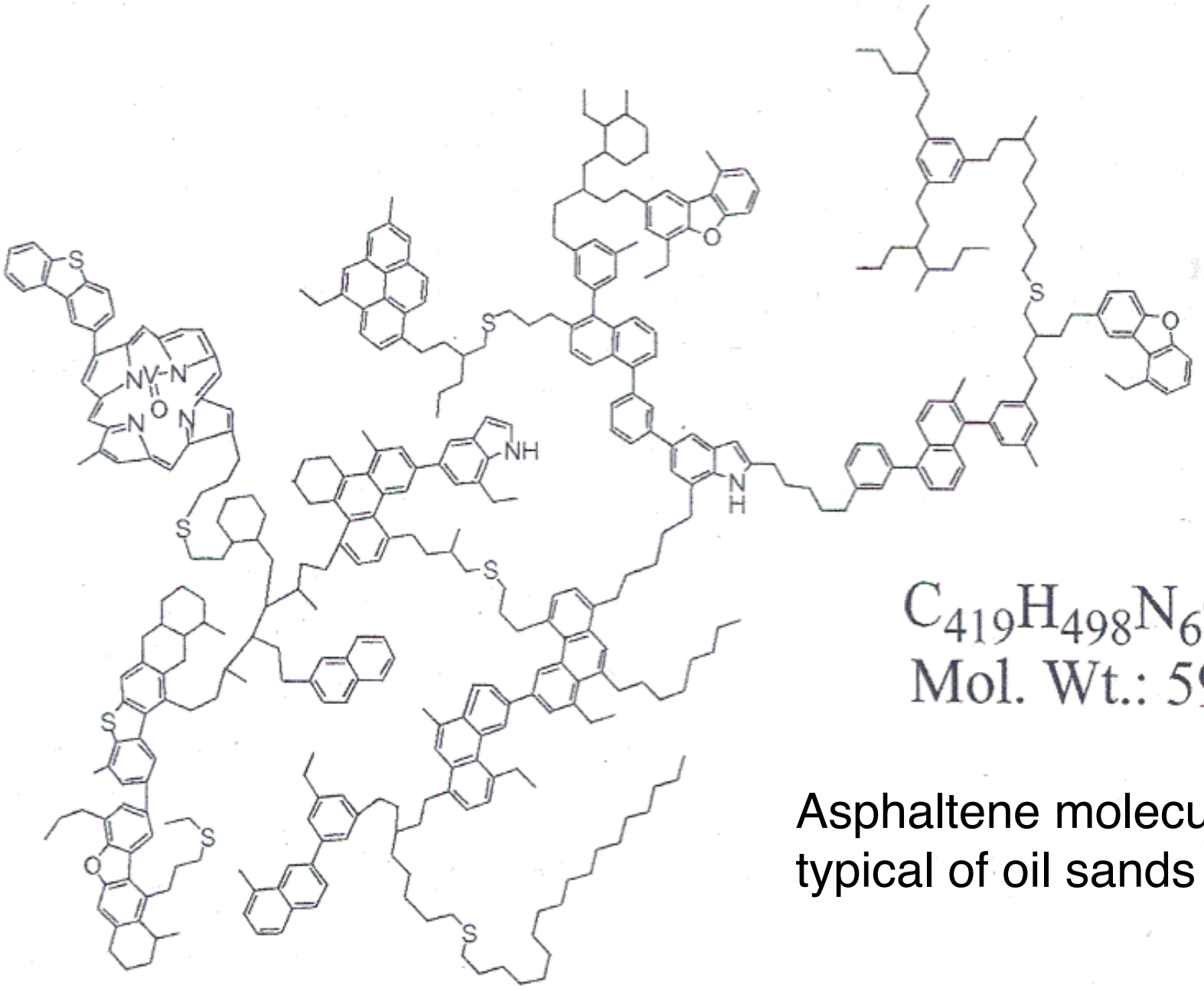
- Conference in Edmonton earlier this month, attended by Canadian and US researchers, emphasis on “upstream” and refining
- US is already blending small fractions of oil sands-derived fuels with diesel fuel
- Concern about combustion characteristics, as well as environmental impacts

Diesel fuels derived from oil sands present combustion challenges that require research

- Derived diesel fuel is rich in cyclic alkanes
  - e.g., methyl cyclohexane



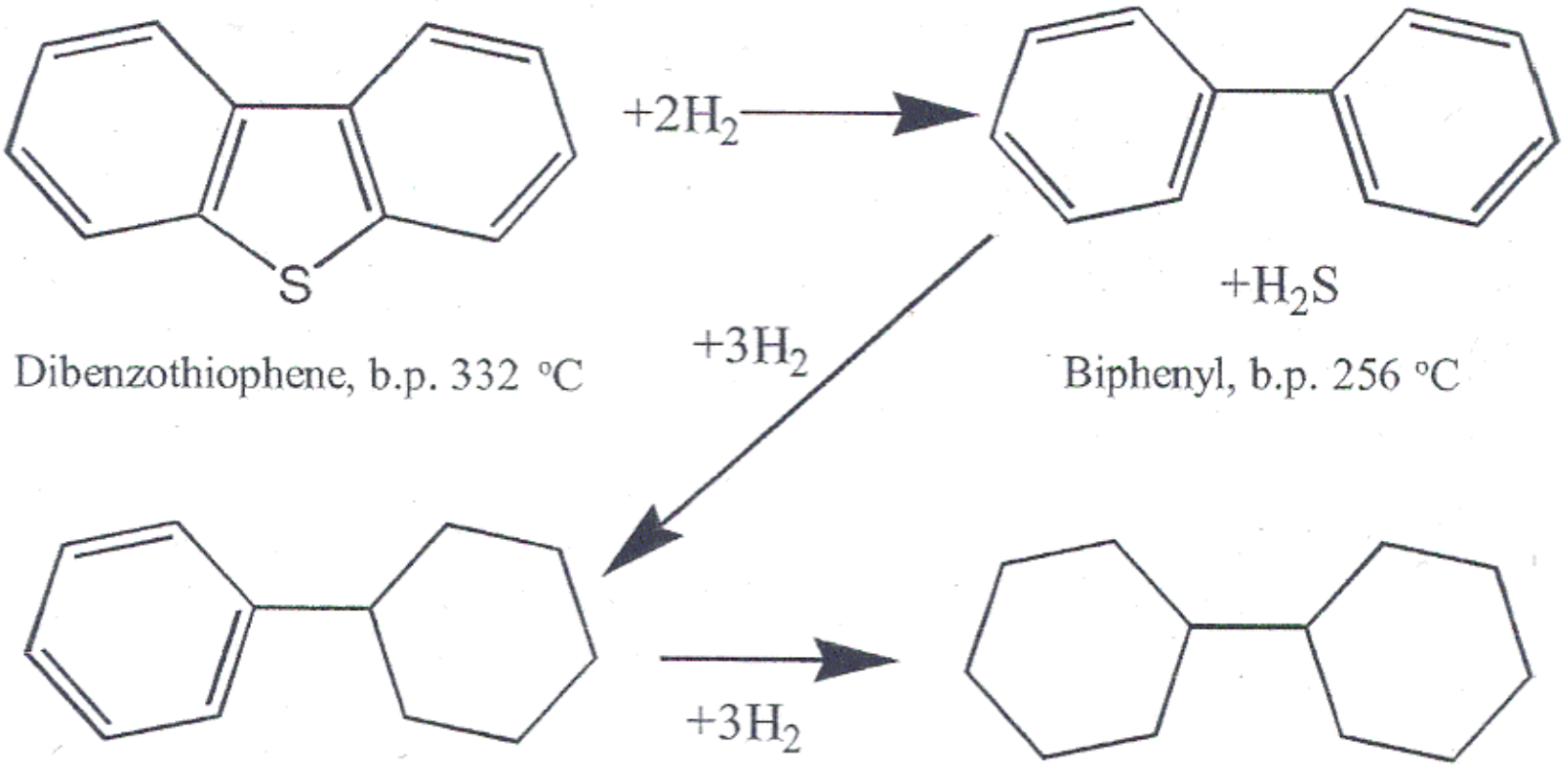
- Most of these are rather large, complex cyclic alkanes
- Very little scientific research has been done on any cyclic alkanes
- Preliminary practical experience suggests that these species are important in determining ignition and soot production in diesels



$C_{419}H_{498}N_6O_4S_8V$
Mol. Wt.: 5989.94

Asphaltene molecule
typical of oil sands

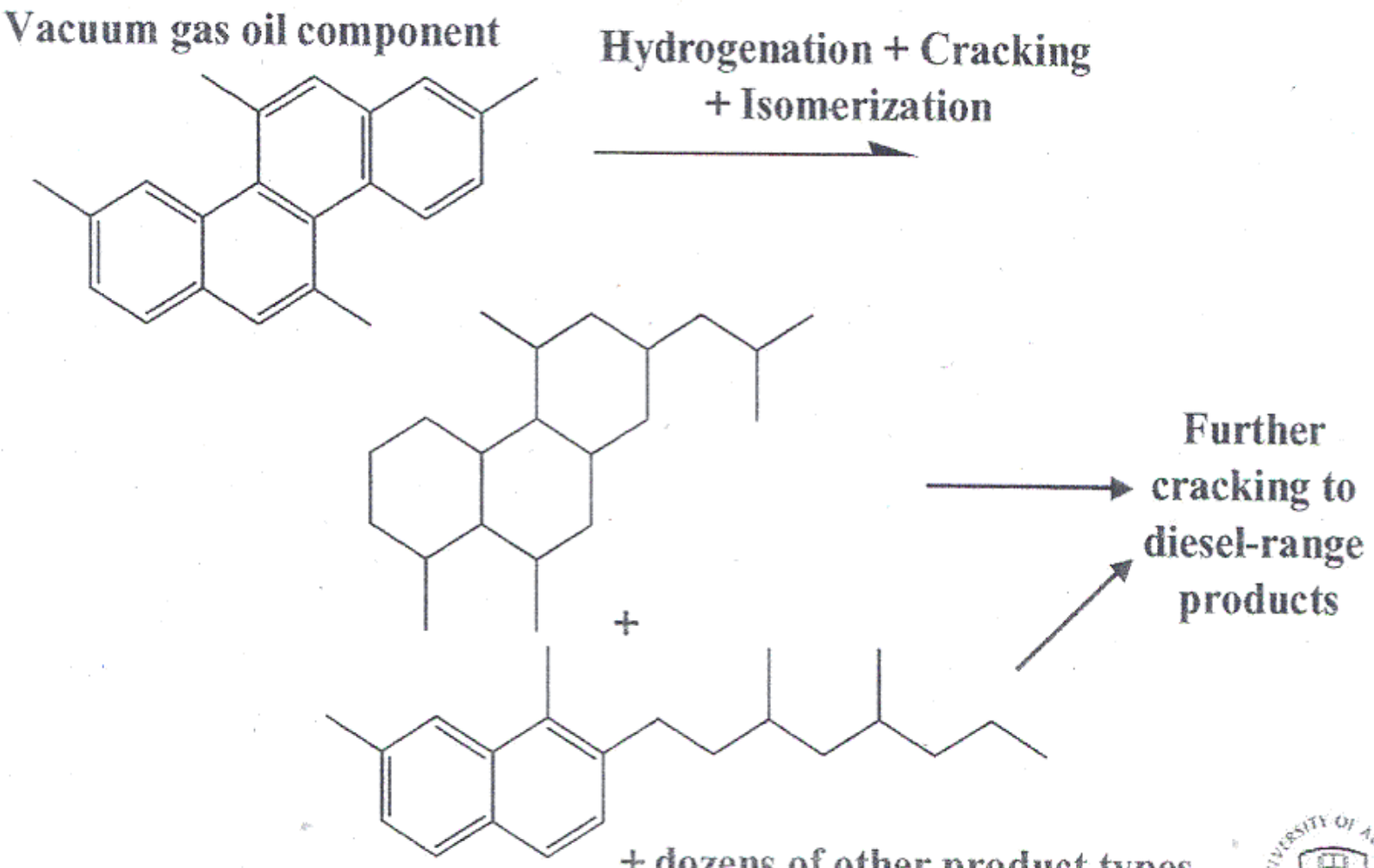
Benefits of Hydrotreating and Aromatic Saturation



Dibenzothiophene, b.p. 332 °C

Biphenyl, b.p. 256 °C

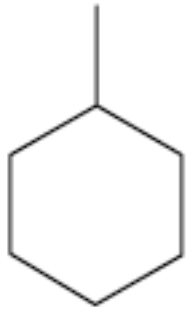
Hydrocracking Gas Oil



After Quann and Jaffe, 1992

The only cycloalkane for which we currently have a good kinetic model is methyl cyclohexane

- How representative is this for actual cycloalkane constituents of fuel composition?



Current answer is: unknown, but further fuel chemistry study is needed

Methyl cyclohexane may be a suitable surrogate for cyclic paraffin hydrocarbons

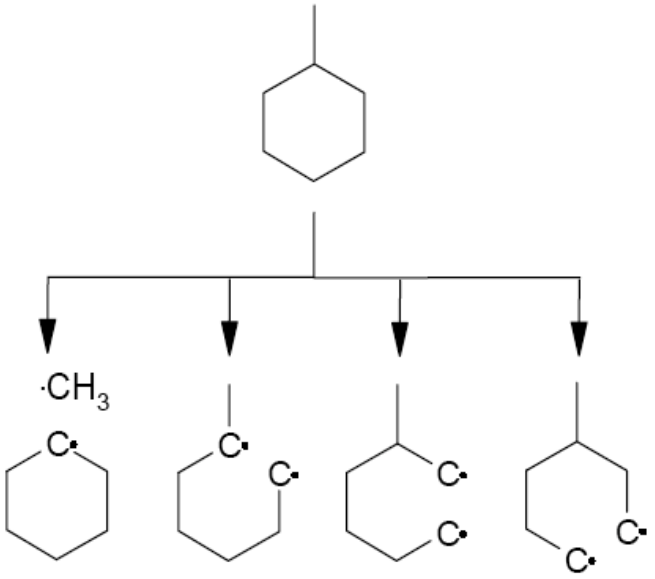


Figure 4: Unimolecular decomposition of MCH

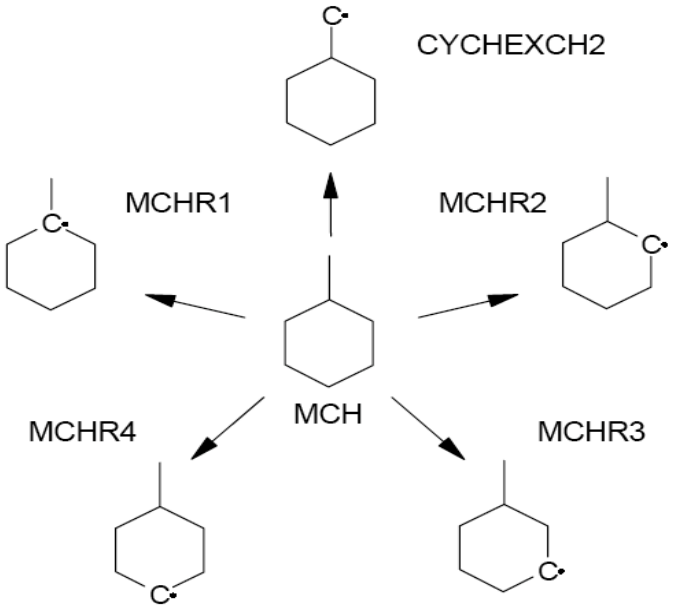
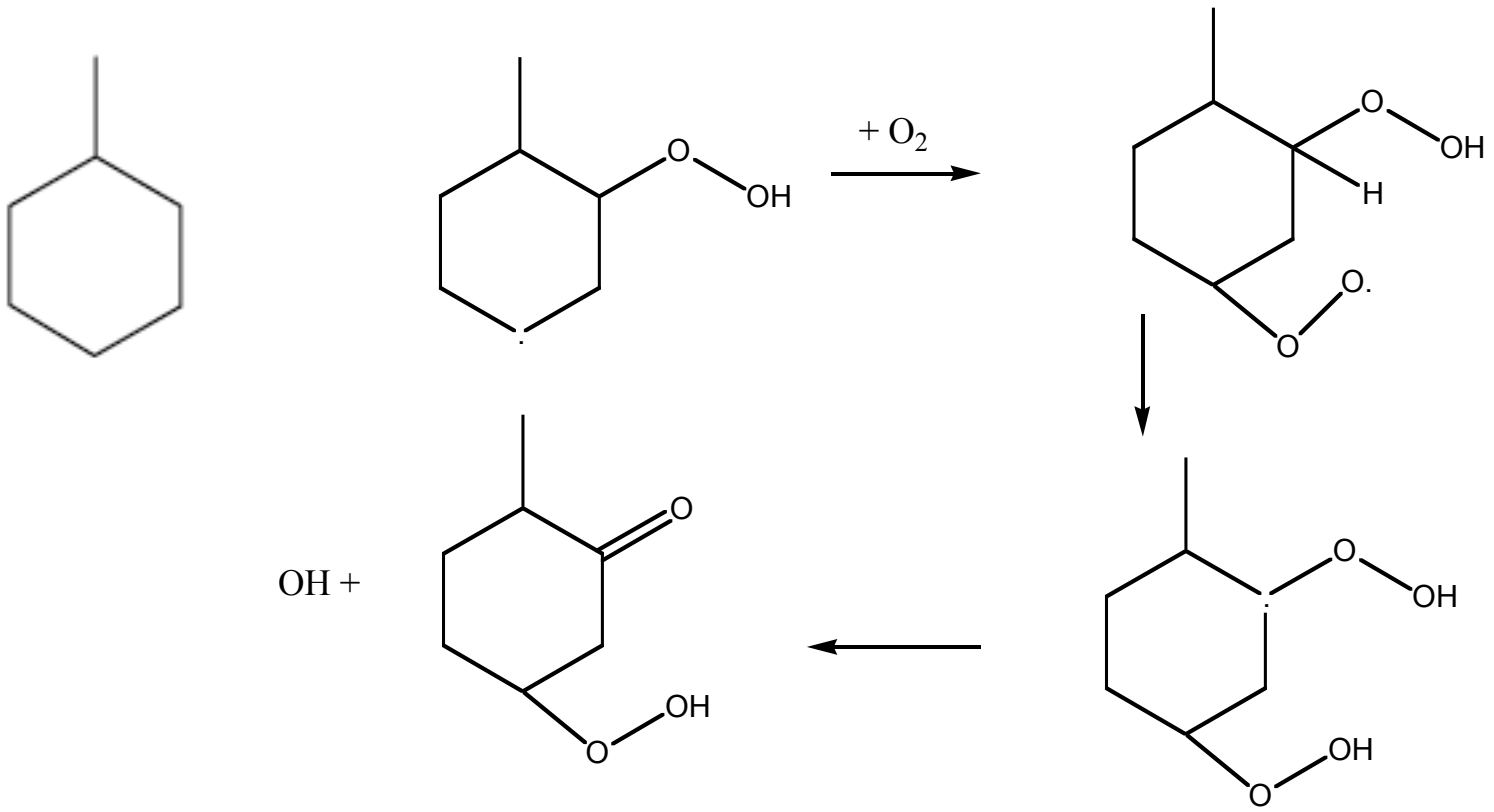


Figure 5: H–atom abstraction from MCH

A mechanism for methyl cyclohexane includes both high and low temperature chemistry

- Estimated thermodynamic parameters for 110 new species and rate constants for 260 new reactions



A start has been made on understanding cycloalkane species combustion

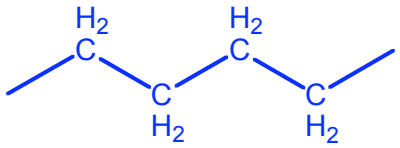
- Sooting and cetane effects of methyl cyclohexane on diesel fuel can be estimated

- Actual fuel composition is much more complex than this simple cycloalkane molecule
  - mixed cycloalkanes and aromatics
  - multicyclic paraffins

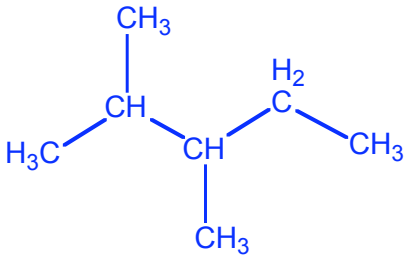
- Lots of chemistry theory, laboratory experiments, and engine experiments will be needed to enable meaningful simulations and impacts on real applications

Classes of hydrocarbons in transportation fuels

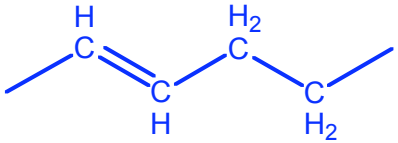
n-paraffin

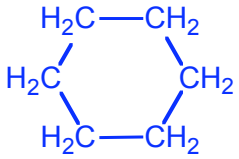


iso-paraffin

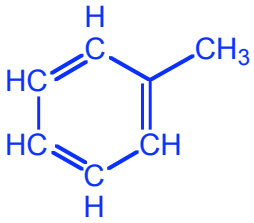


olefin

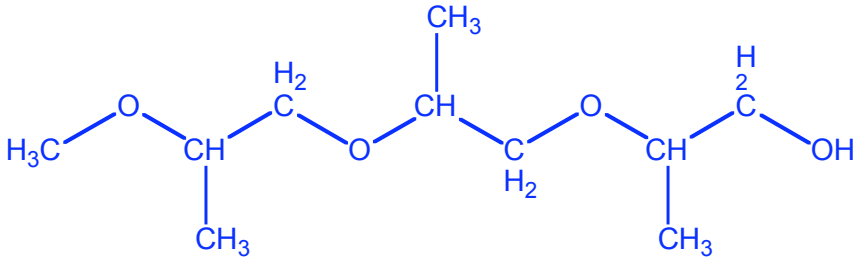




cyclo-alkane



aromatic



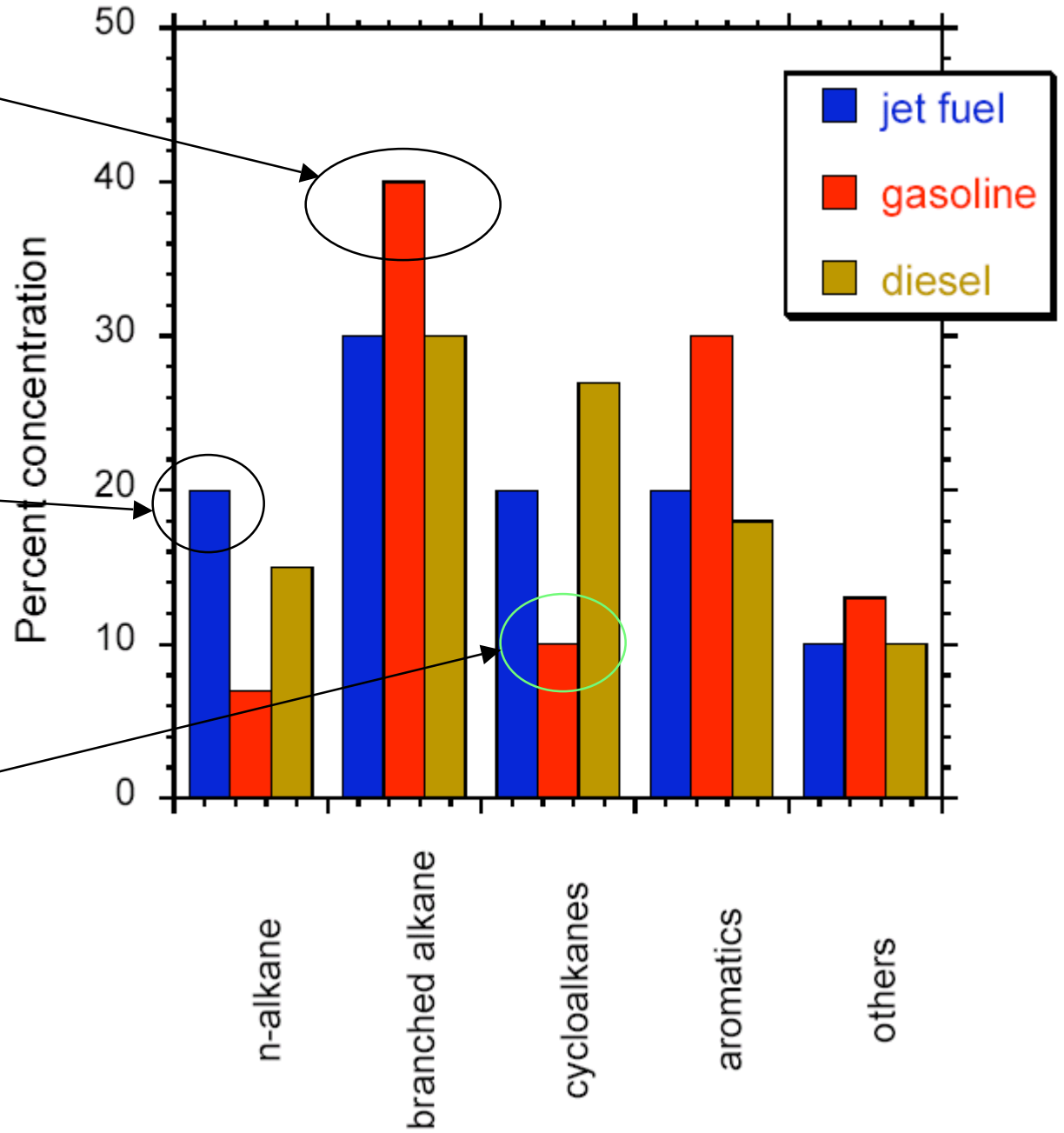
oxygenate

Each class has unique combustion characteristics

Gasoline has many branched alkanes

Jet fuel has the highest n-alkane

Gasoline is lower in cycloalkanes



Variability of real transportation fuels

- Composition of gasolines at different gas stations on a single day is often quite different
- Composition of same gas station will vary every day
- Same is true of diesel and jet fuels
- Quantity used to test fuels is often not very demanding or specific (e.g., ON, CN)

Example:
levels of different hydrocarbons in samples of 3 types of jet fuel (JP-8, Jet A and JP-5)

Iso-Nonene	4.00	8.73	2.06
2,2,4-Trimethyl Hexane	0.00	1.46	0.00
2,3,5-Trimethyl Hexane	6.41	5.20	2.49
2,2-Dimethyl Heptane	7.22	0.00	0.00
cis 1,2-Dimethyl Cyclohexane	3.32	13.66	5.37
2,4-Dimethyl Heptane	29.10	4.90	3.75
Iso-Nonene	32.04	22.11	11.47
Iso-Nonene	43.24	30.41	17.23
Unidentified	6.28	5.71	1.75
Ethyl Cyclo-Hexane	266.85	175.68	140.31
2-Methyl-4-Ethyl Hexane	3.50	2.03	0.00
2,6-Dimethyl Cyclohexane	91.75	61.64	47.64
Iso-Nonene	0.00	8.35	0.00
1,1,3-Trimethyl Cyclohexane	88.04	105.67	64.05
Nonene	25.45	20.80	10.54
2,5-Dimethyl Heptane	86.97	46.78	23.50
Iso-Nonene	34.41	9.67	6.26
Iso-Nonane	0.00	13.95	6.48
3,3-Dimethyl Heptane	10.84	25.34	11.52
Iso-Nonene	5.26	14.82	6.01
Ethyl Benzene	105.97	74.18	70.47
1,2,4-Trimethyl Cyclohexane	15.52	32.00	20.47
Isononene	65.71	83.73	30.32
2,3,4-Trimethyl Hexane	3.48	5.60	4.72
Isononene	2.48	0.00	0.00
3,3,4-Trimethyl Cyclohexane	3.43	10.54	1.63
meta-Xylene	439.45	134.95	160.21
para-Xylene	124.56	45.32	47.37
2,3-Dimethyl Heptane	69.23	38.37	35.94
3,5-Dimethyl Heptane	8.73	6.46	3.60
3,4-Dimethyl Heptane	39.46	21.67	19.49
3-Methyl-3-Ethyl Hexane	18.52	19.40	8.82
Isononene	2.54	7.41	2.96
4-Methyl Octane	88.02	65.70	37.01
2-Methyl Octane	117.21	87.71	49.14
Iso-Nonane	17.61	17.20	11.67
3-Ethyl Heptane	36.82	45.69	20.15
3-Methyl Octane	126.82	130.04	64.67
1,2,4-Trimethyl Cyclohexane	0.00	3.21	2.66
1,1,2-Trimethyl Cyclohexane	0.00	13.38	0.00
ortho-Xylene	235.28	82.34	112.71
Isononene	0.00	14.75	10.17
Isononene	1.73	17.32	5.58
Isononene	3.79	3.65	1.69
Isononane	22.13	47.40	33.14
1-Ethyl-4-Methyl Cyclohexane	90.36	98.14	58.69
Isononane	73.47	60.57	43.02
Nonene-1	1.85	8.98	6.97
Isobutyl Cyclopentane	6.51	17.66	9.59
Isononane	0.00	1.70	0.00
cis Nonene-3	22.68	10.99	9.51
Isononane	0.00	4.60	1.77
n-Nonane	449.86	313.15	290.63
trans Nonene-2	60.82	78.13	47.69
Isononene	4.16	0.00	30.68
1-Methyl-2-Propyl Cyclopentane	31.60	24.13	23.01
C10 Iso-paraffin	0.00	0.00	3.68
Isopropyl Benzene	22.23	19.95	26.85
t-Butyl Pentane	2.25	2.86	0.00
Isononene	7.92	11.35	6.15
Isononene	44.66	56.22	49.60
Isopropyl Cyclohexane	40.39	37.42	36.42
2,2-Dimethyl Octane	29.59	32.22	19.33
2,4-Dimethyl Octane	27.45	20.14	16.91
Isodecane	0.00	6.38	1.50
1-Methyl-4-Isopropyl Cyclohexane	3.65	2.71	2.67
s-Butyl Cyclopentane	13.08	28.59	13.99
2,6-Dimethyl Octane	23.57	28.04	11.37
2,5-Dimethyl Octane	74.50	78.06	79.83
Isodecane	10.88	21.48	11.69
Butyl Cyclopentane	12.93	17.87	6.46
Propyl Cyclohexane	22.75	35.18	26.79
Isodecane	0.00	16.27	9.11
3,5-Dimethyl Octane	51.42	89.34	70.09
1-Methyl-2-Ethyl Cyclohexane	24.76	18.15	20.74
Isodecane	6.83	6.11	8.63
Isodecene	5.57	29.31	10.88
n-Propyl Benzene	55.70	70.21	69.12
3,6-Dimethyl Octane	36.82	63.33	50.22
3-Methyl-5-Ethyl Heptane	0.00	12.57	6.60
Isodecene	6.33	18.01	10.24
Isodecene	5.11	11.47	5.66
meta Ethyl Toluene	83.33	72.54	74.71
para Ethyl Toluene	46.13	64.58	50.25
1,3,5-Trimethyl Benzene	123.63	140.06	111.93
2,3-Dimethyl Octane	3.20	14.85	1.40
Isodecane	1.81	22.95	13.16
5-Methyl Nonane	19.22	48.92	21.85
4-Methyl Nonane	37.93	85.43	54.49
2-Methyl Nonane	41.16	91.11	53.04
ortho Ethyl Toluene	23.71	26.83	43.66
3-Ethyl Octane	3.78	3.73	4.12
Napthene	9.86	28.20	13.57
Isodecane	2.44	5.22	9.43
Isodecane	2.28	0.00	0.00
3-Methyl Nonane	48.31	105.77	66.17
Isodecane	0.00	23.16	20.20
Isodecene	8.04	10.99	3.79
Isodecane	15.59	31.17	26.52
Isodecane	4.82	14.17	8.20
1,2,4-Trimethyl Benzene	103.36	116.35	114.54
Isodecane	18.85	41.84	33.94
Isodecane	11.77	33.82	33.89
Isodecane	18.24	42.34	40.71
Isobutyl Cyclohexane	1.98	16.90	10.48
Isodecane	4.34	7.71	9.02
Isodecane	2.22	14.52	10.88
Decene-1	2.23	8.96	7.61
Isodecane	1.75	2.41	3.42
C10 Aromatic	5.74	18.07	14.39
Napthene	14.80	23.20	28.46
1-Methyl 2-Propyl Cyclohexane	0.00	3.76	0.00
n-Decane	179.98	281.60	379.89
Iso-undecane	0.00	2.06	2.14
Iso-undecane	2.26	1.71	3.24
Iso-undecane	0.00	5.59	2.35
Iso-undecane	1.51	1.87	1.81
1,2,3-Trimethyl Benzene	43.58	55.87	77.07
Iso-undecane	4.98	15.21	16.31
para-Isopropyl Toluene	8.90	13.40	20.89
Iso-undecane	8.34	26.23	23.52
Iso-undecane	2.33	5.65	5.32
Iso-undecane	1.07	8.14	6.66
Indan	13.49	34.27	30.80
Iso-undecane	2.24	7.84	10.14
Isobutyl Cyclohexane	34.20	87.01	130.81
Iso-undecane	0.00	0.00	2.35
Iso-undecane	2.31	1.72	3.64
ortho-Isopropyl Toluene	6.94	19.90	15.78

A 5-component surrogate can represent gasoline

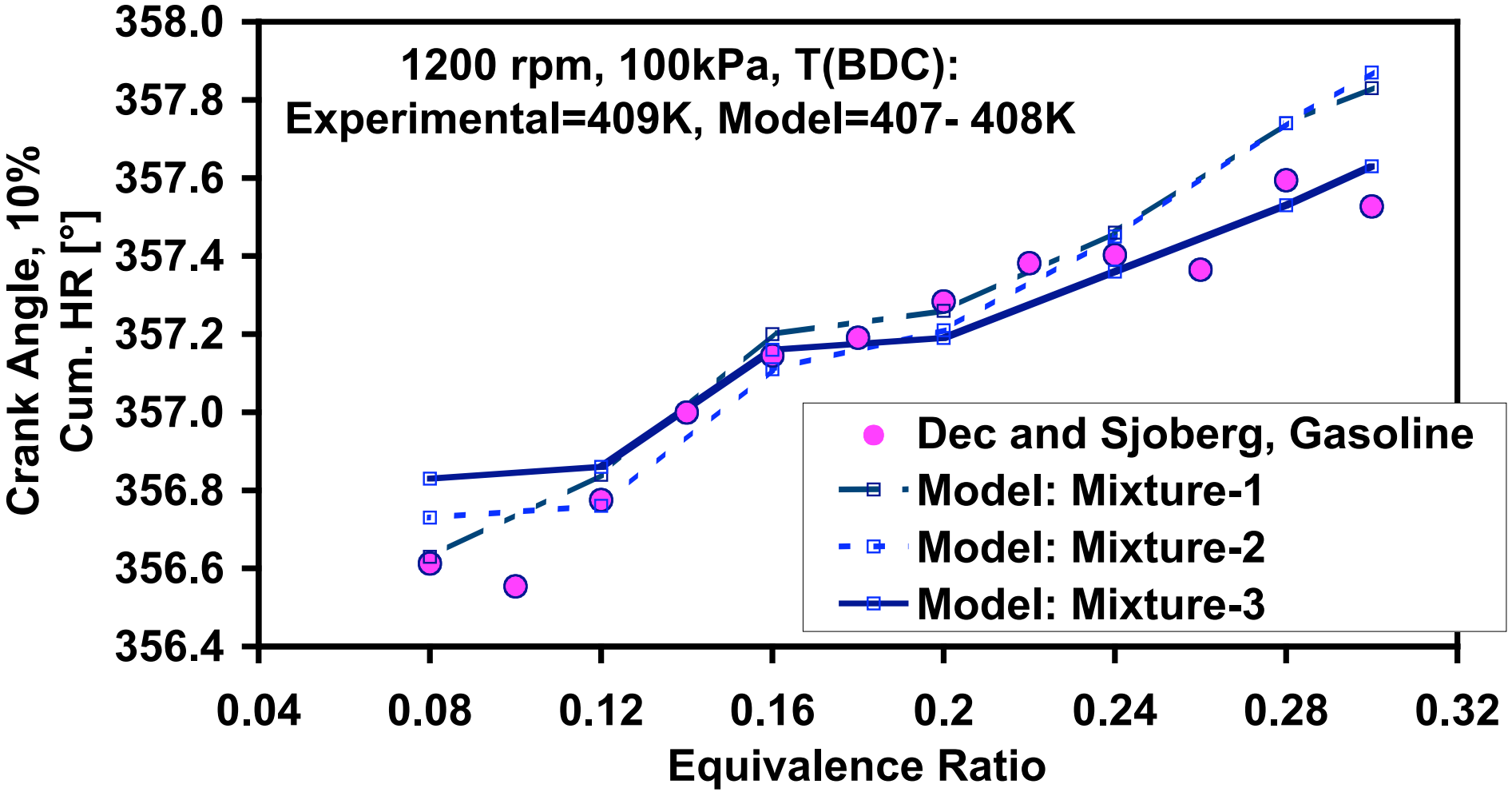
- n-heptane (straight chain alkanes)
- iso-octane (branched alkanes)
- 1-pentene (alkenes)
- toluene (aromatics)
- methylcyclohexane (cycloalkanes)
- One representative of each fuel class

Surrogate fuel compositions examined:

- Mixture 1: Five components to represent the different classes of compound in gasoline at the typical level.
- Mixture 2: Match the octane number of gasoline based on *blended* octane numbers.
- Mixture 3: Increase the low temperature chemistry by adding more n-heptane

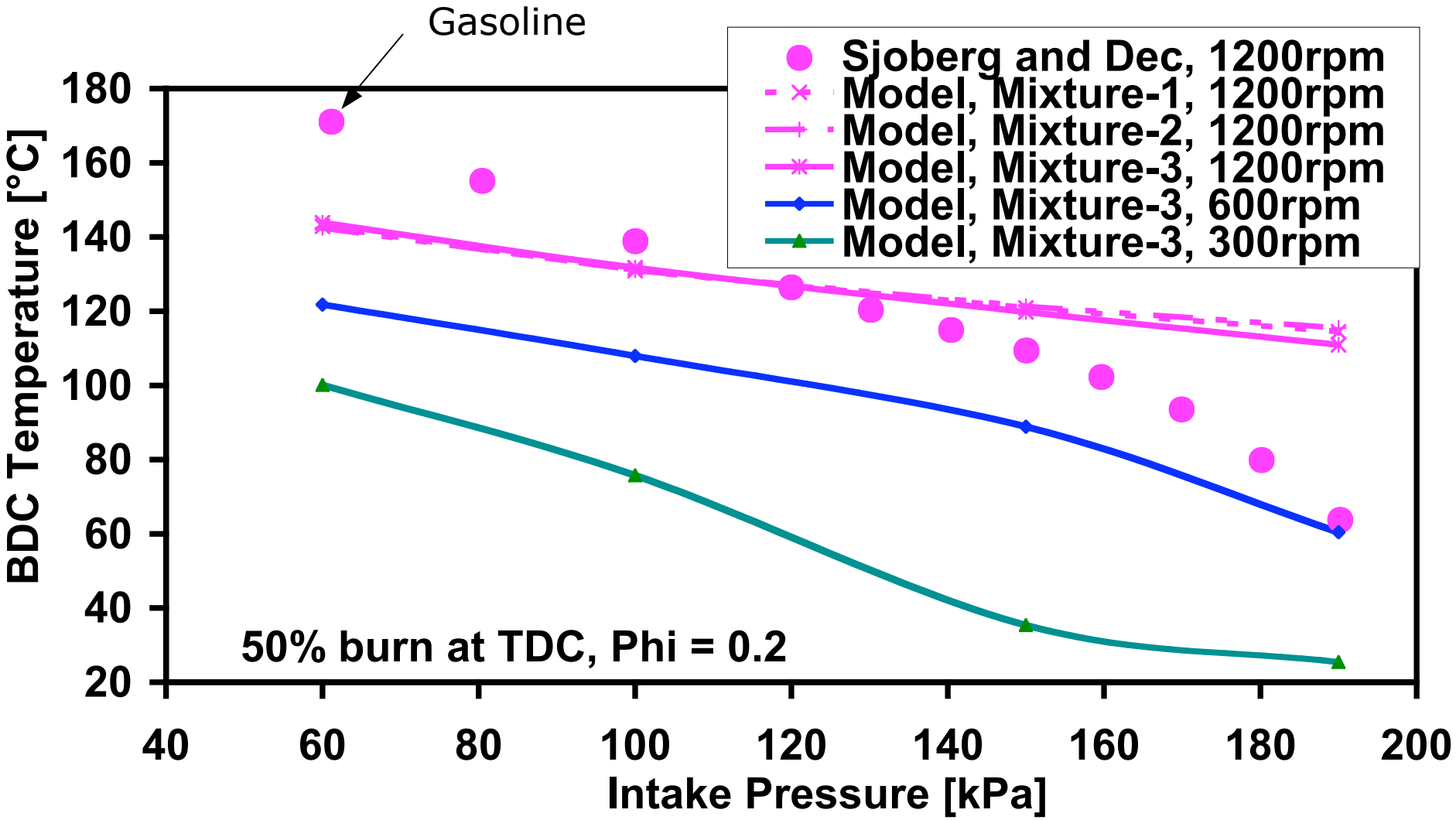
% molar composition	Mixture 1	Mixture 2	Mixture 3
iso-Octane	60	40	40
n-Heptane	8	10	20
Toluene	20	10	10
Methyl cyclohexane	8	40	30
1-Pentene	4	0	0
RON (linear)	93.7	81.7	83.7
MON (linear)	90.6	79.3	79.8
RON (blend)	99.2	94	87.6
MON (blend)	94.5	84.8	82

Effect of equivalence ratio on timing for start of combustion



Effect of intake pressure on temperature required to maintain TDC timing:

effects of pressure on kinetics are not yet correct



Comparisons to shock tube data on gasoline surrogates:

Stanford data: Gauthier, Davidson and Hanson, Combust. Flame 139 (2004) 300-311

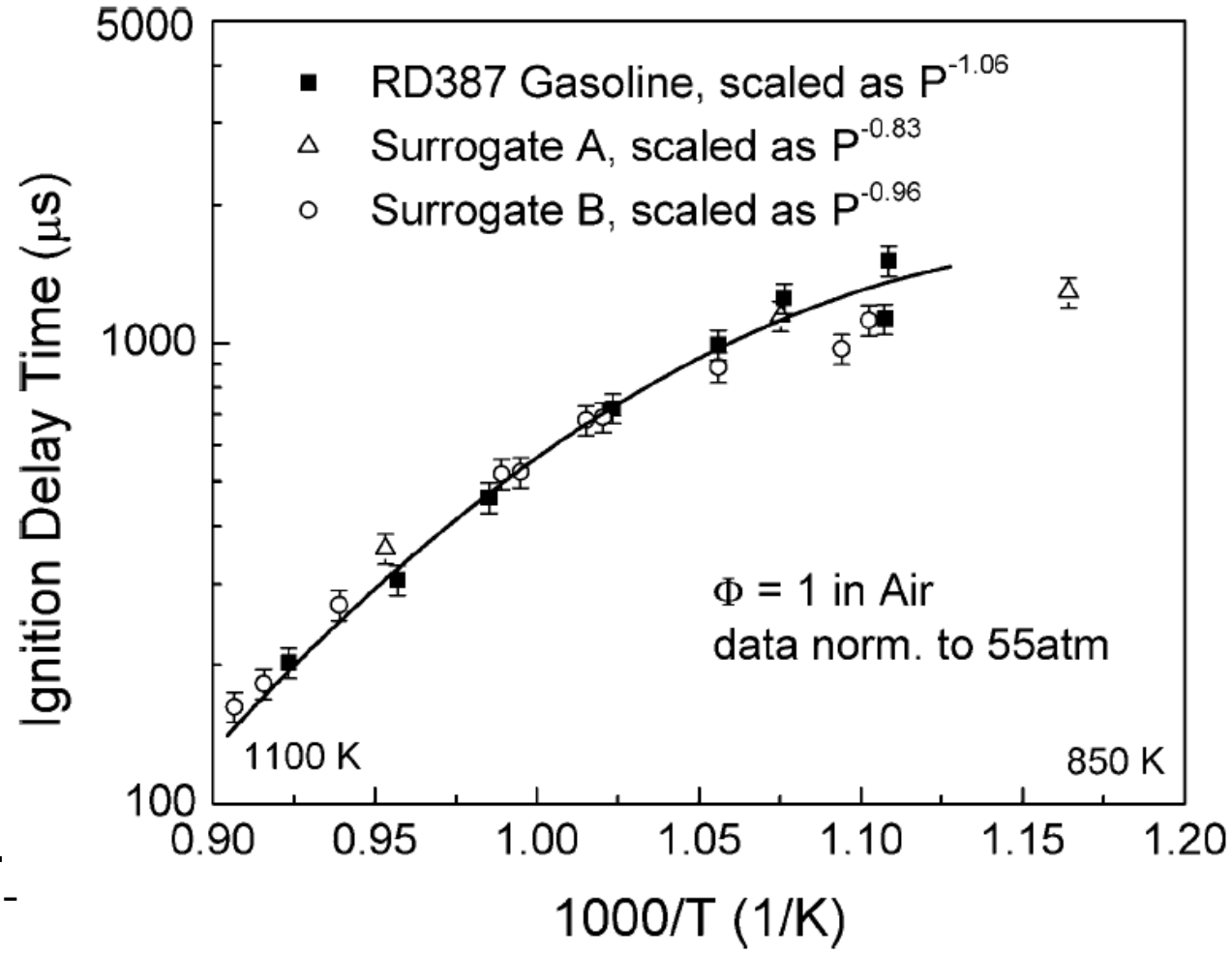
- RD387 Gasoline (GM Research)
- Surrogate A:

  63% iso-octane/20% toluene/17% n-heptane

- Surrogate B:

  69% iso-octane/14% toluene/17% n-heptane

Both surrogates A and B compare well with gasoline under shock tube conditions



(Gauthier, Davidson and Hanson, Combust. Flame 139 (2004) 300-311)

More detail is needed for surrogate fuels

- Next aromatics are naphthalene and xylene
- Next cycloalkanes are ethyl cyclohexane, cyclopentane, and multicyclic alkanes
- Include diisobutylene as additional olefin
- Include multiple species in each of the 5 or 6 classes of fuels in a given surrogate
- Need suitable surrogates for each practical fuel

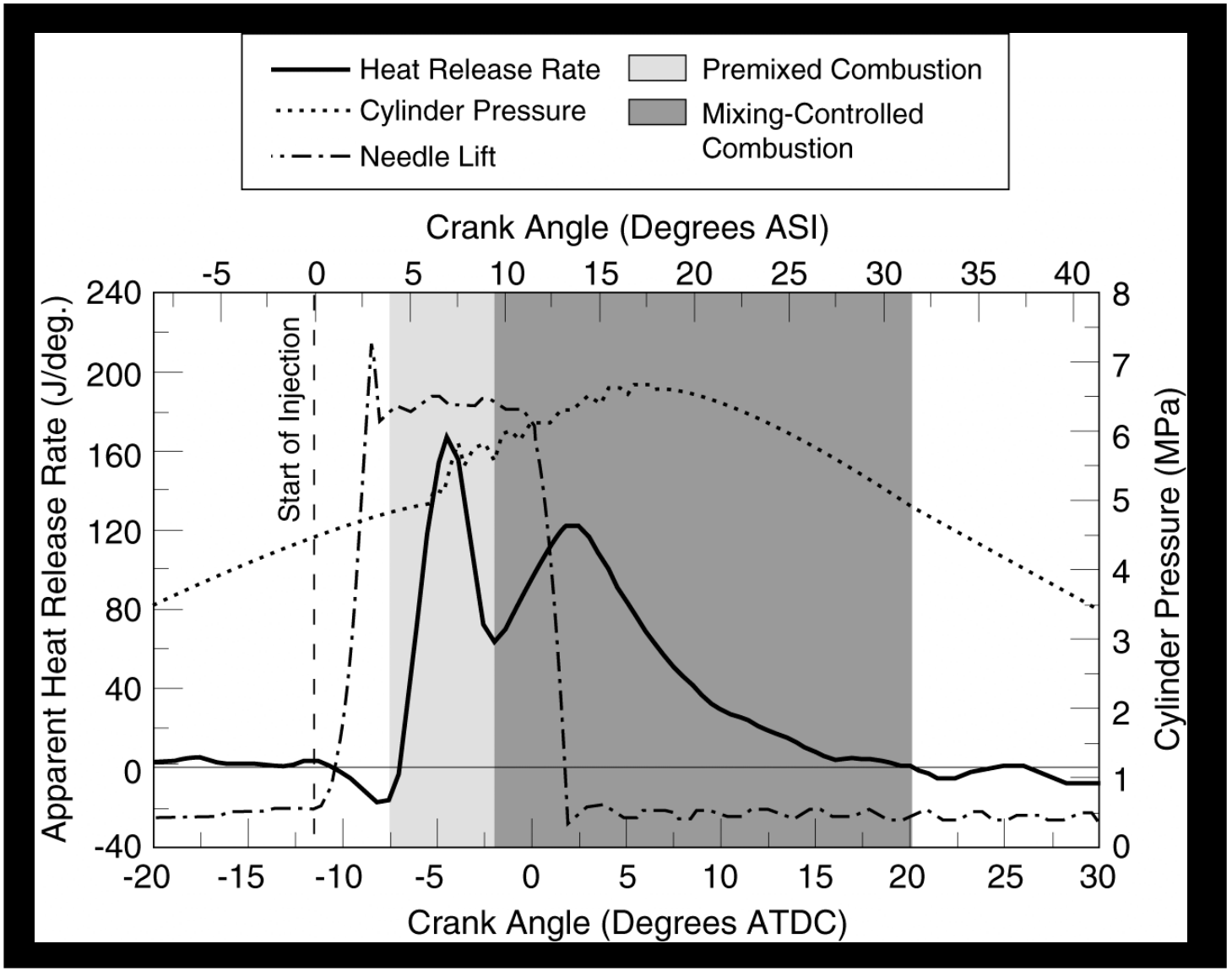
  diesel, gasoline, jet fuel, natural gas, etc.
- Need different surrogate for same fuel in different applications

  gasoline in SI engines, HCCI engines

Constituents of surrogate fuels

- Each species requires basic research
- Each species needs experimental data over a wide range of experimental parameters
  - shock tubes
  - flow reactors
  - rapid compression machines
- Each species requires kinetic modeling research, thermochemistry
- These are major research tasks

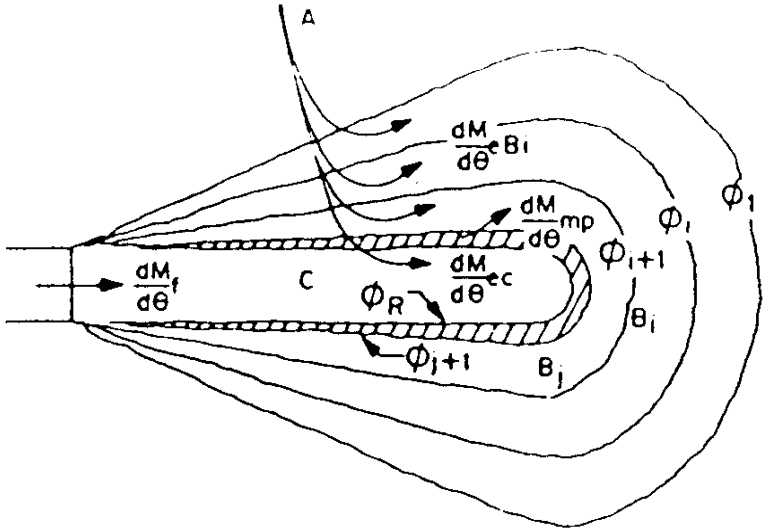
Diesel engine combustion: A revolution



Early models of Diesel combustion

Liquid core with air continuously entrained

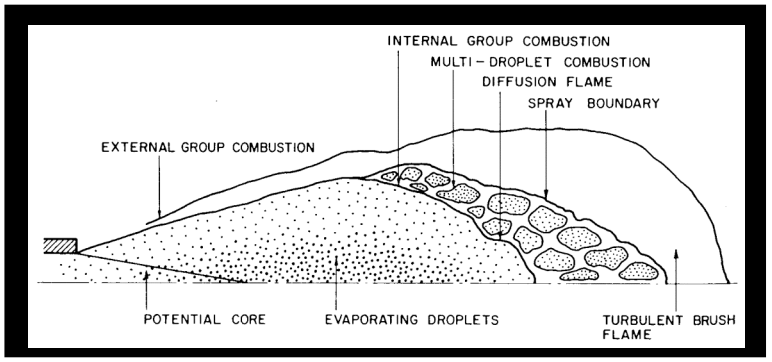
Chou (1976)



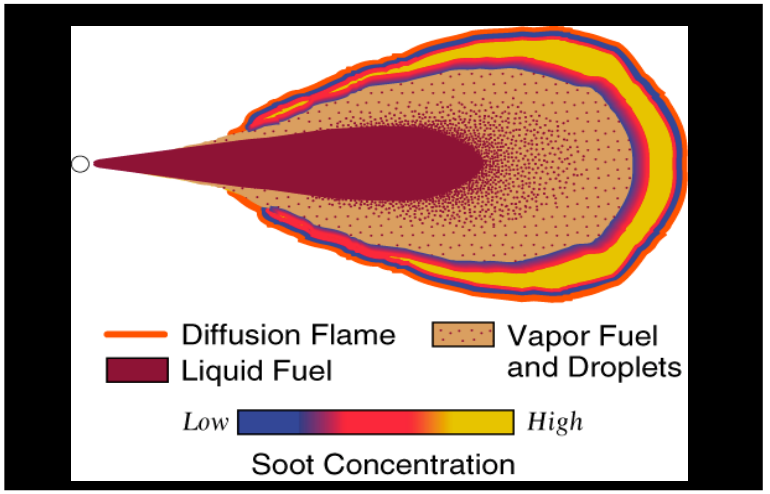
Prior to Laser-Sheet Imaging

- Autoignition and premixed burn were thought to occur in near-stoichiometric regions.
- The "quasi-steady" portion of Diesel combustion was thought to be adequately described by steady spray combustion theory.
- Appeared to fit most available data.
- This "old" description was never fully developed into a conceptual model.

  A "representative" schematic is given.



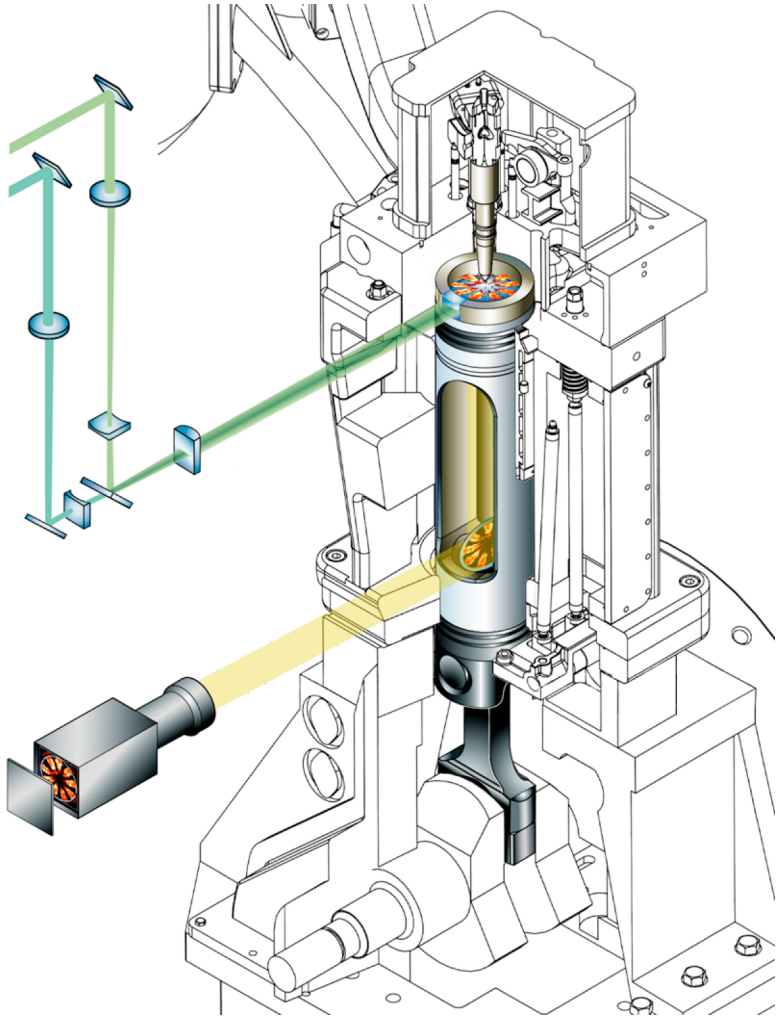
Schematic of group combustion for a fuel spray.
From Kuo, as adapted from H. Chiu and Croke



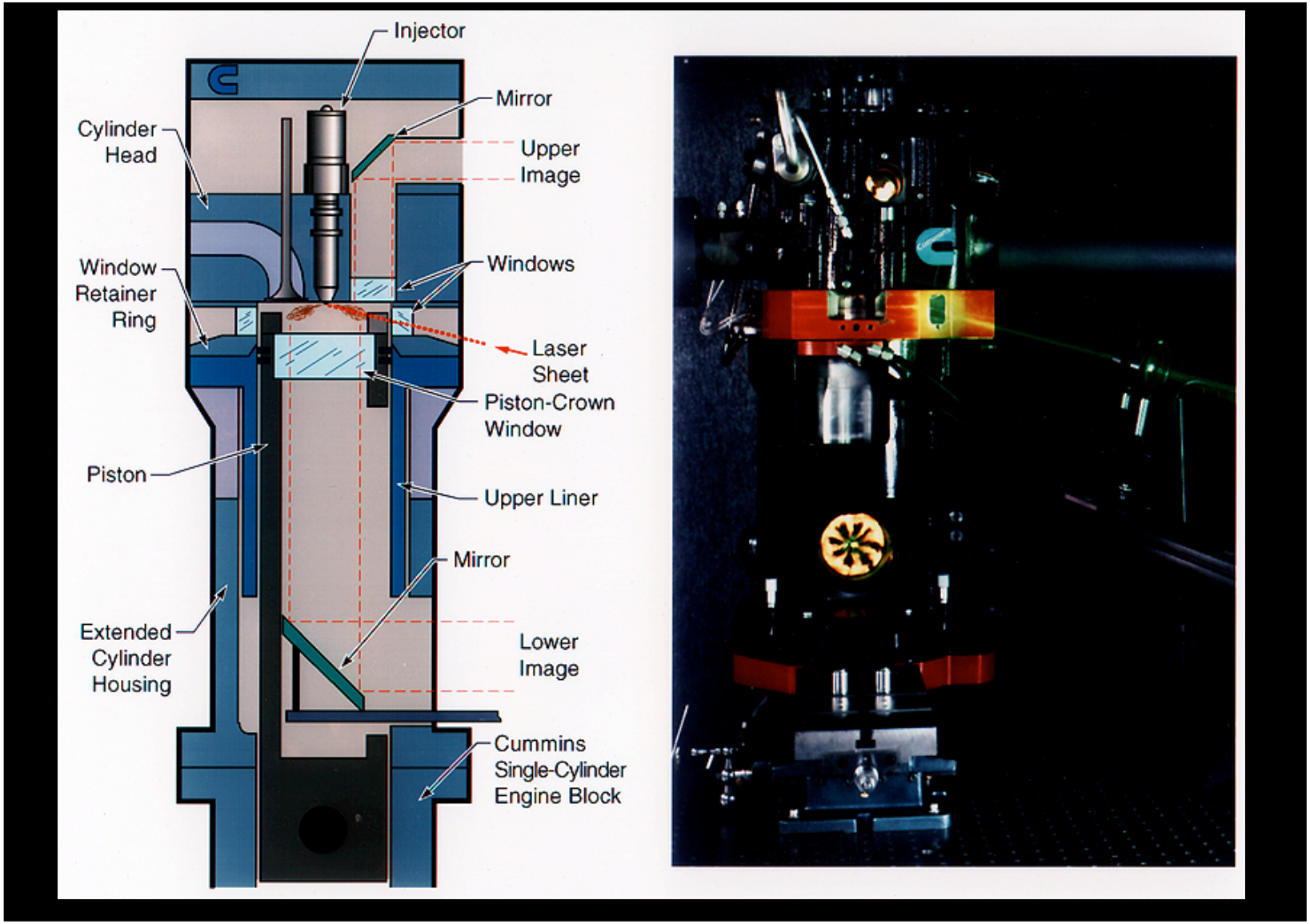
Old description of DI Diesel combustion.

The DOE Engine Combustion Research Program at Sandia's CRF played a major role in solving the diesel "mystery".

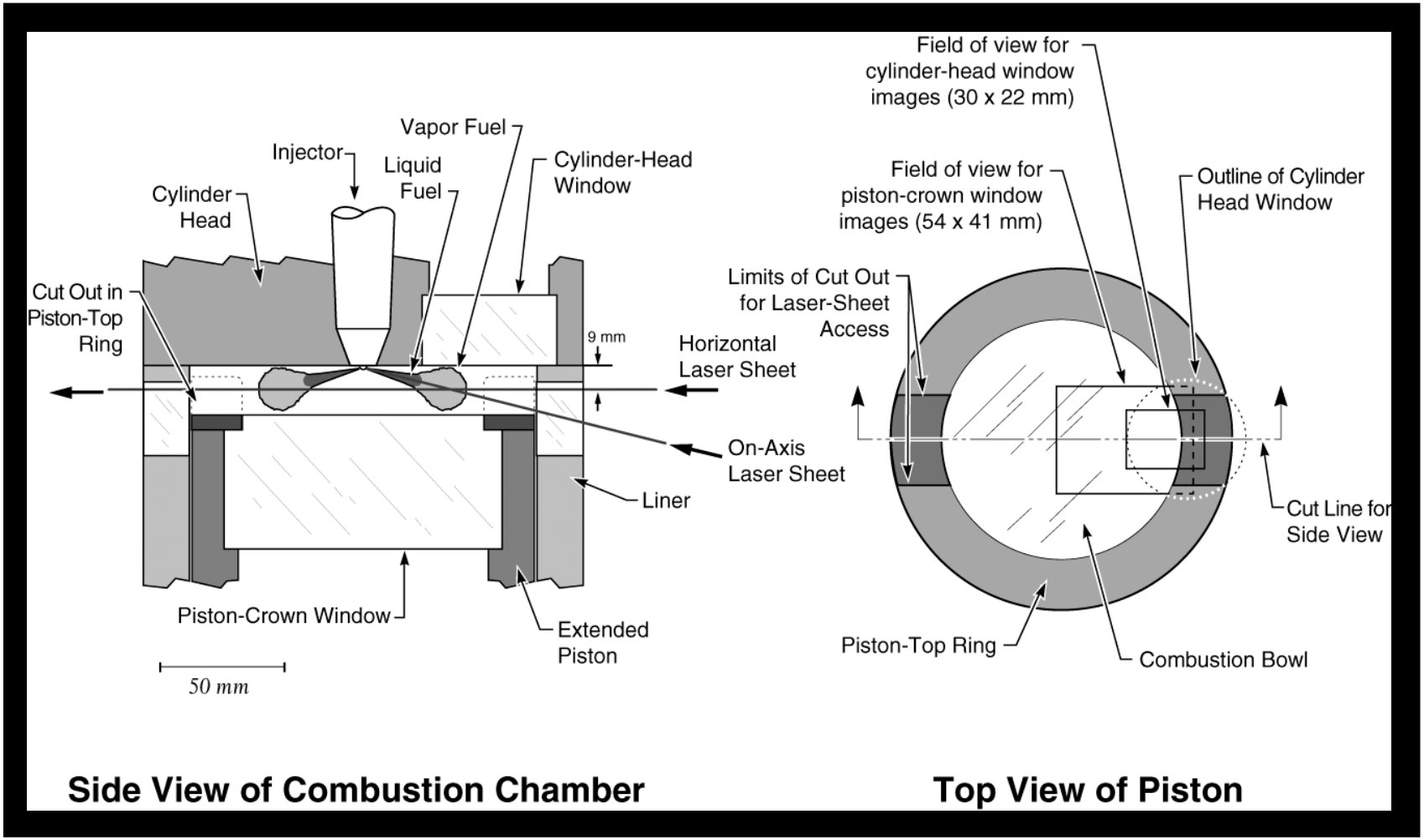
- ***Mission*** - Develop the science-base for in-cylinder combustion and emissions processes.
  - Help U.S. manufacturers reduce emissions & improve performance.
- ***Approach*** –
  - Strong interaction and collaboration with industry.
  - Optical diagnostics.
  - Realistic engine geometries with optical access through:
    - *pistons*
    - *cylinder liner*
    - *spacer plates*
    - *exhaust ports*



Sandia/Cummins Diesel Engine

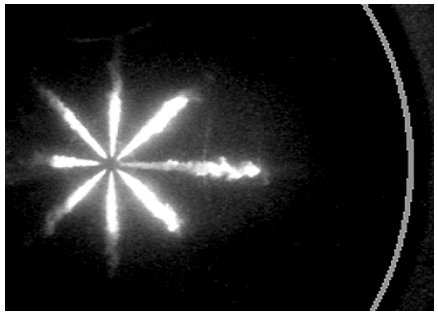


Optical Setup



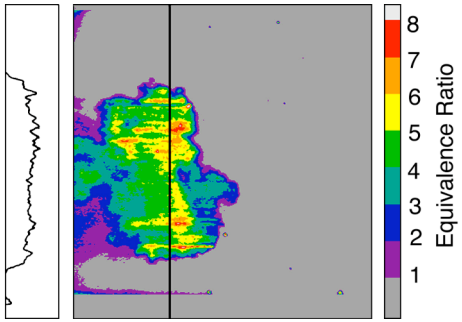
Laser-Sheet Imaging Data - 1

Liquid-phase Fuel



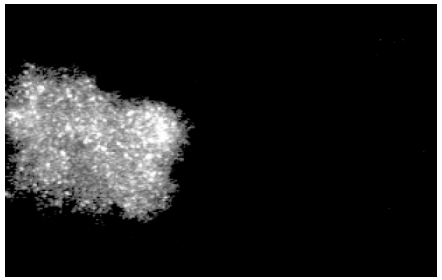
- Liquid fuel images show that all the fuel vaporizes within a characteristic length (~1 inch) from the injector.

Vapor-phase Fuel



- Vapor fuel images show that downstream of the liquid region, the fuel and air are uniformly mixed to an equivalence ratio of 3-4.

Chemiluminescence

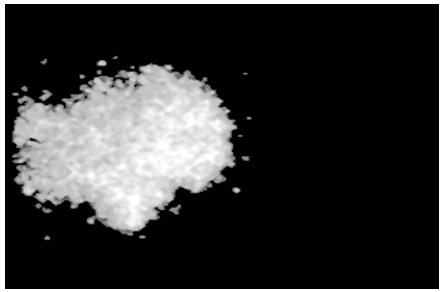


- Chemiluminescence images show autoignition occurring across the downstream portion of the fuel jet.

Quiescent Chamber, 1200 rpm, T_{TDC} = 1000 K, ρ_{TDC} = 16.6 kg/m^3

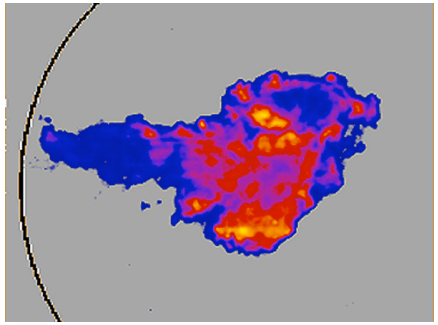
Laser-Sheet Imaging Data - 2

PAH Distribution



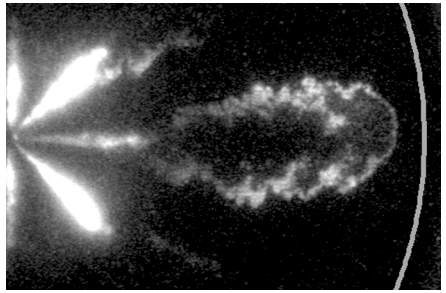
- PAHs form throughout the cross-section of the fuel jet immediately following fuel breakdown at the start of the apparent heat release.

Soot Distribution



- LII soot images show that soot forms throughout the cross-section of the fuel jet beginning just downstream of the liquid-fuel region.

OH PLIF Image



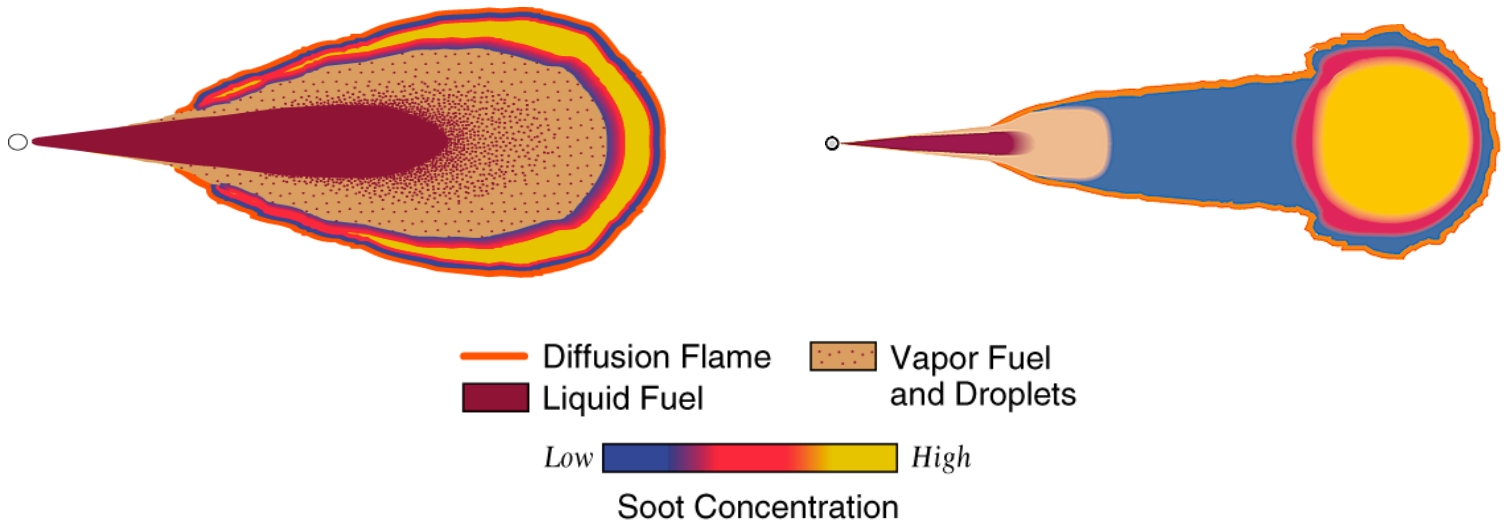
- OH radical images show that the diffusion flame forms at the jet periphery subsequent to an initial fuel-rich premixed combustion phase.

Quiescent Chamber, 1200 rpm, T_{TDC} = 1000 K, ρ_{TDC} = 16.6 kg/m^3

Laser Sheet Imaging is Providing a New Understanding of DI Diesel Combustion

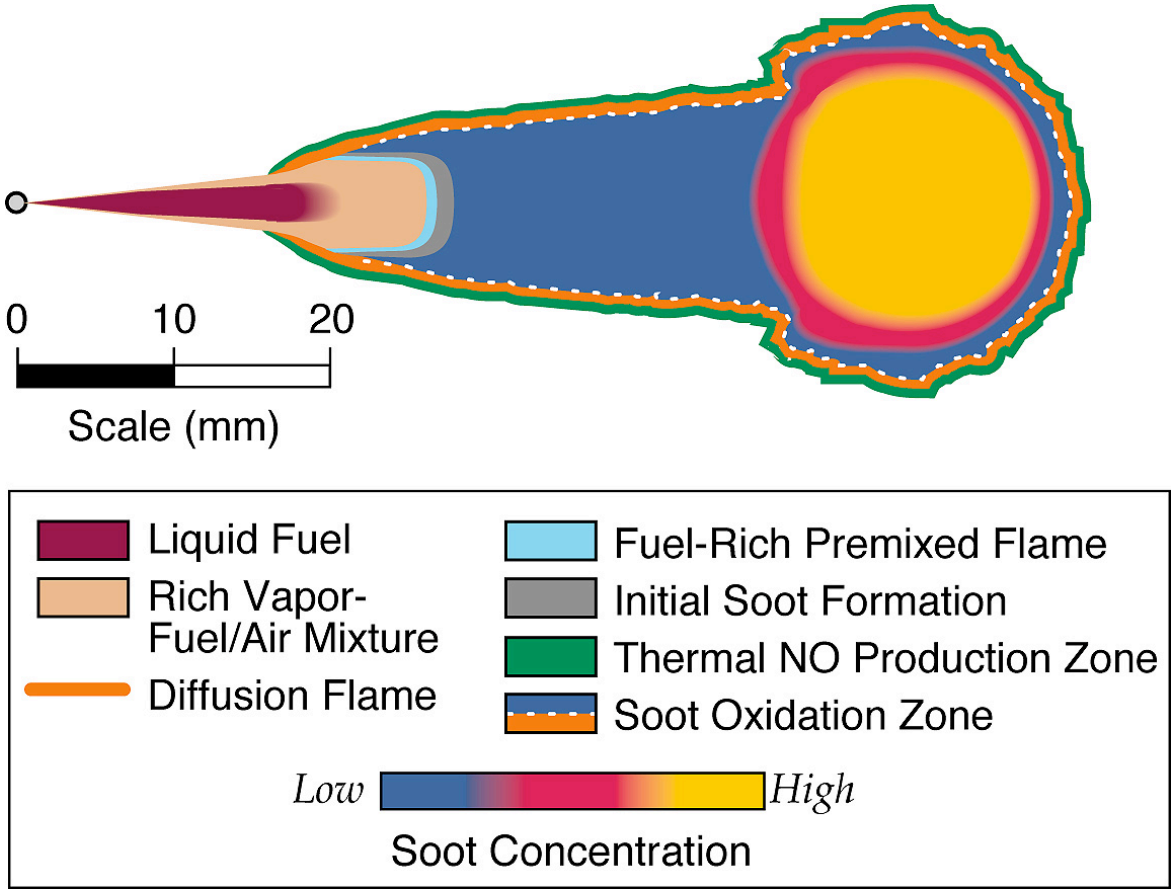
Old Description

New Conceptual Model

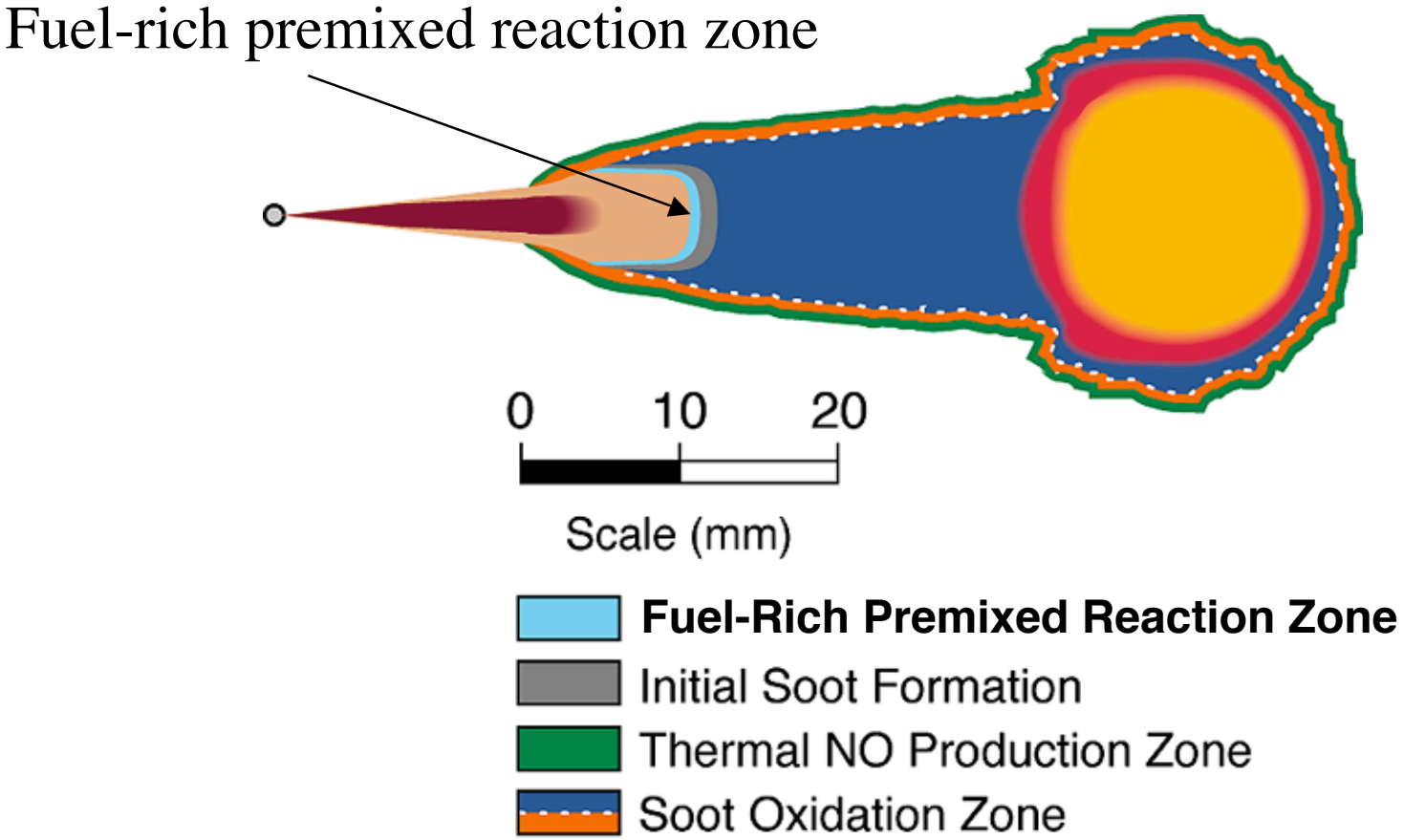


- The appearance is significantly different.
  - Regimes of Diesel combustion are different than thought. (flame standoff, upstream mixing, instantaneous vs. averaged).

Typical Schematic:
First Part of Mixing-Controlled Burn



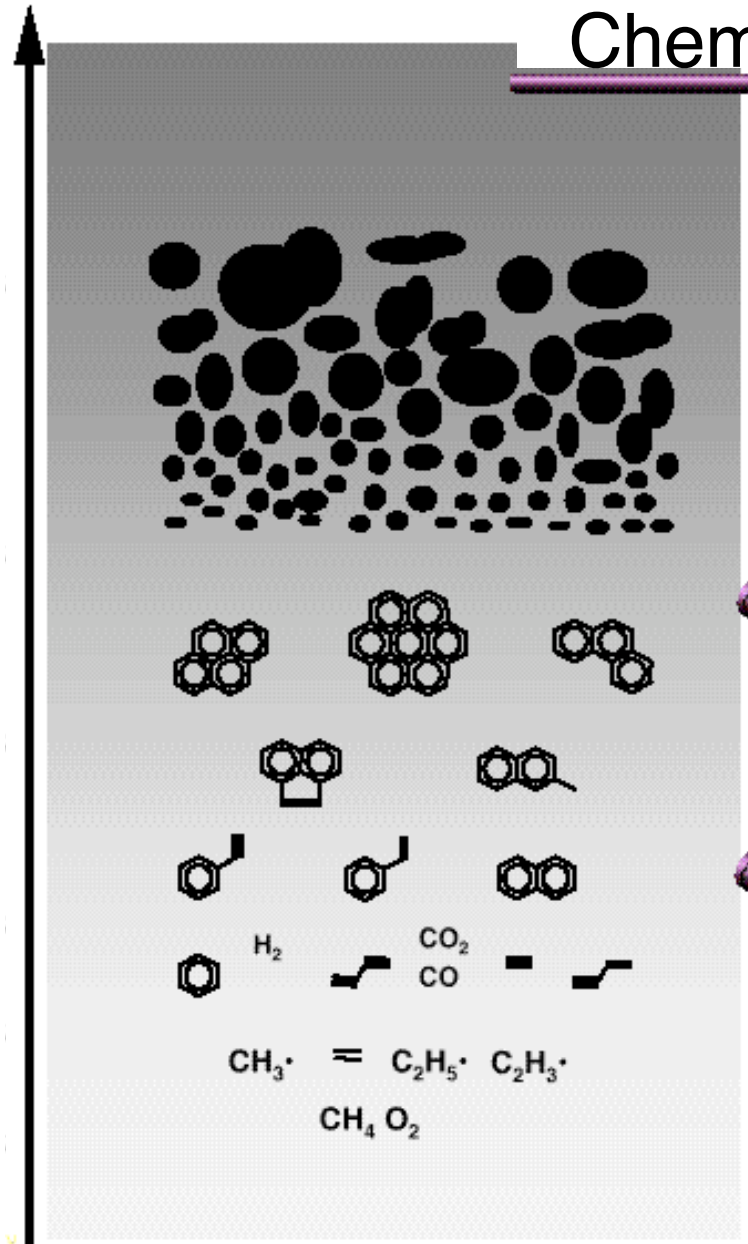
Predicting the soot precursors is one of the keys to predicting soot emissions from a Diesel engine



Premixed ignition in Diesel combustion

- Fuel-rich conditions ($\Phi \approx 4$)
- Relatively low temperature ($T \approx 850$ K)
  - Source of cetane ratings in Diesel engines
  - Very similar to conditions of engine knock
  - Very complex chemical kinetic pathways
- Products are good producers of soot precursor species
- Ignition kinetics are the same as in engine knock in SI engines, driven by H_2O_2 decomposition

Chemical evolution of soot



- oxidation
- agglomeration
- growth
- inception/nucleation

particle zone

$C_9H_7 + C_5H_5 = C_{12}H_8 + H + H$

$C_{10}H_7 + C_2H = C_{12}H_8$

molecular zone

$C_8H_7 + C_2H_2 = C_{10}H_8 + H$

$C_3H_3 + C_3H_3 + THIRD = C_6H_6 + THIRD$

$OH + C_2H_4 = C_2H_3 + H_2O$

$C_2H_6 = C_2H_4 + H_2$

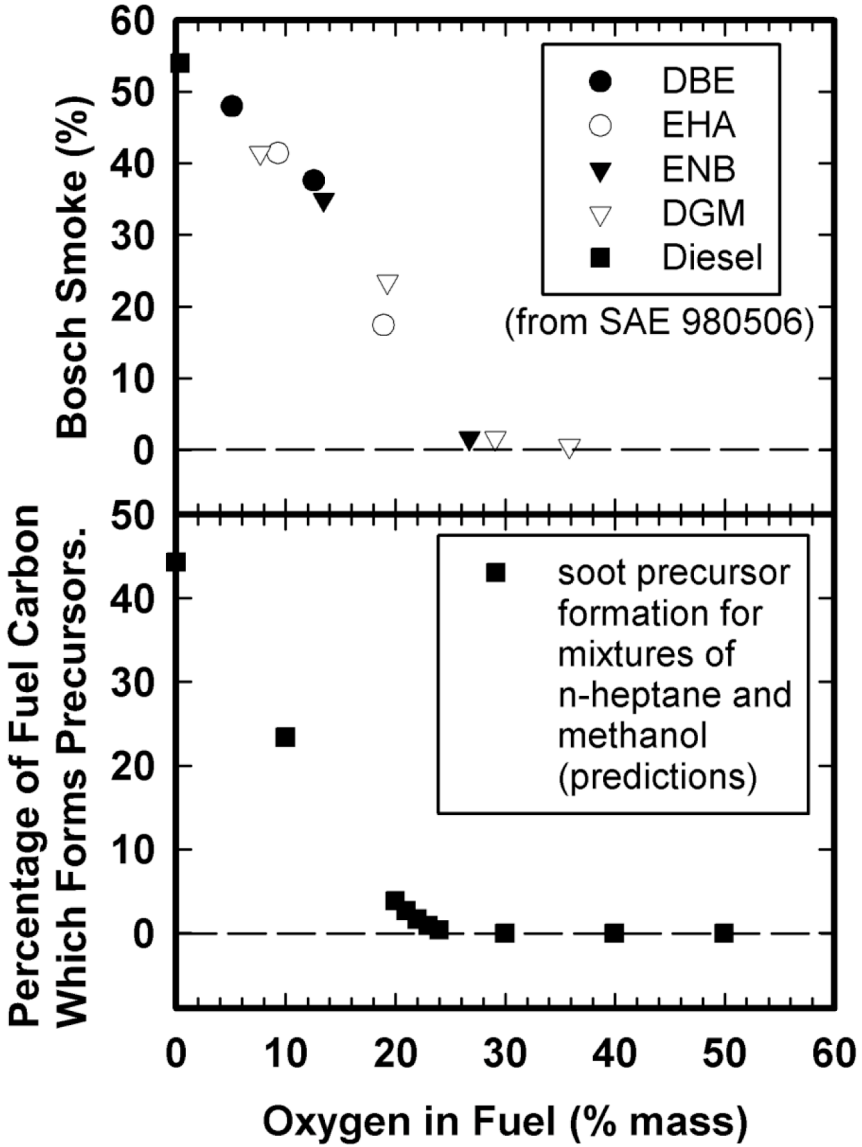
$CH_4 + O_2 = CH_3 + HO_2$

$CH_4 + THIRD = CH_3 + H + THIRD$

Experimental background

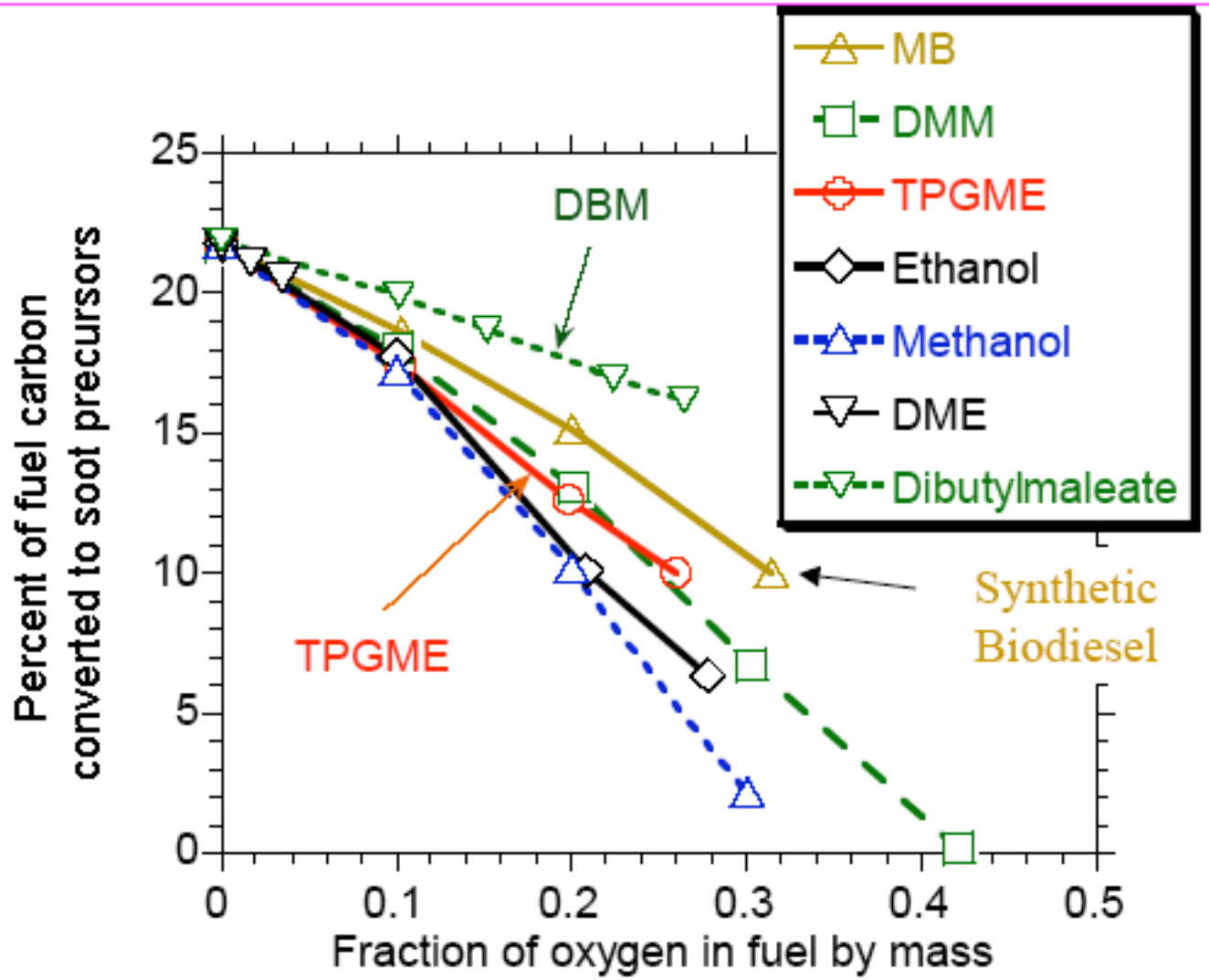
- Addition of oxygenated species reduces soot
  - Important possible oxygenates include biodiesel fuels
- Soot production correlates with post-ignition levels of selected chemical species
- Suggestions that this is due to presence of C - C bonds or total O concentrations
- Use kinetic model to examine these possibilities

Predicted level of soot precursors correlates well with soot emissions from a Diesel engine

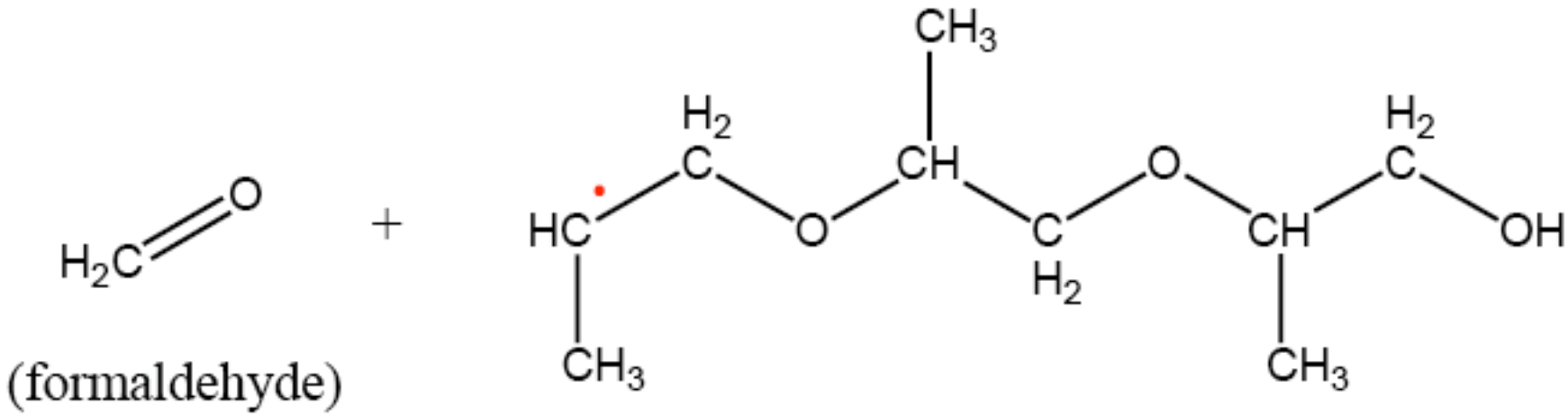


From:
Flynn, Durrett, Dec, Westbrook, et al., SAE paper 1999-01-0509

How well an oxygenated fuel works depends on its molecular structure



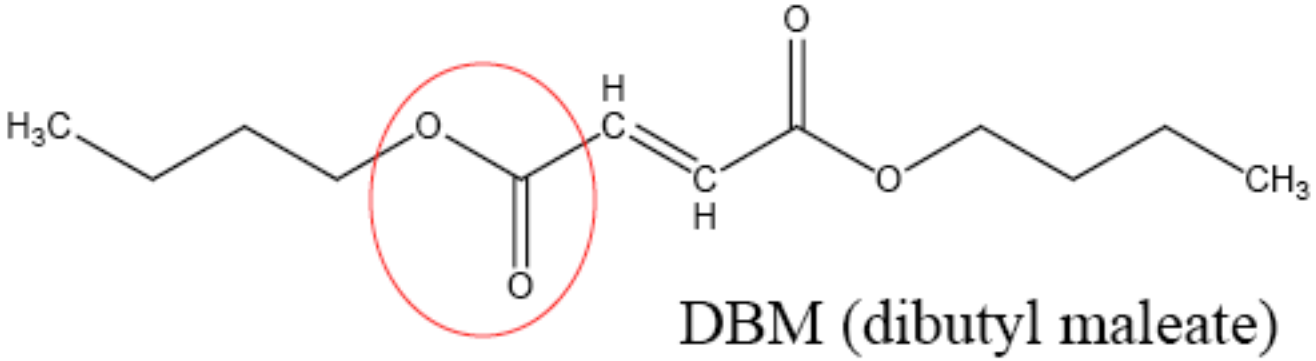
As the oxygenate is consumed, ideally each O atom should stay attached to one C atom to make CO



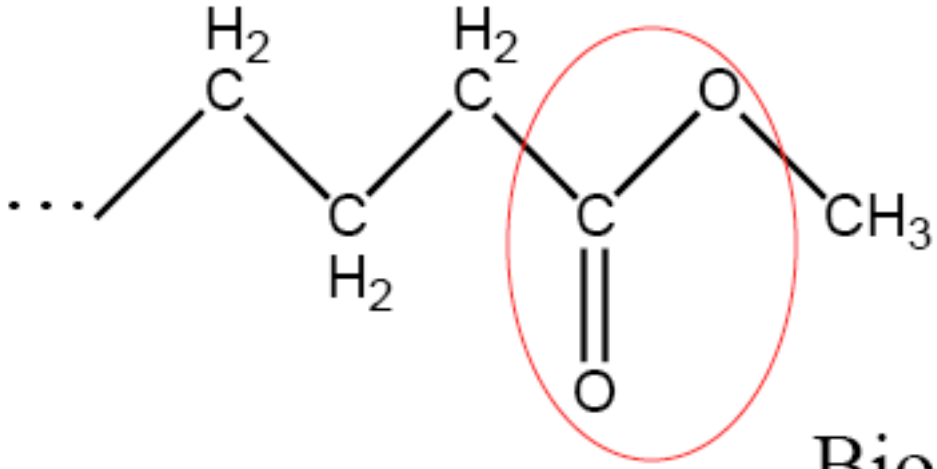
(formaldehyde)

Goes to CO

One large group of oxygenates have ester structures where one carbon atom is attached to two oxygen atoms



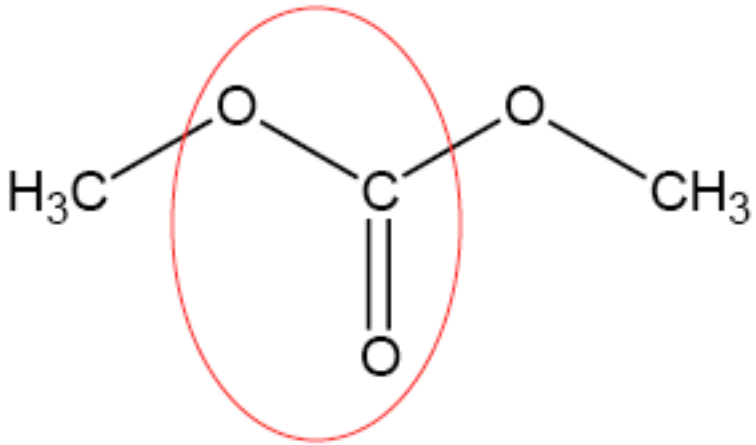
DBM (dibutyl maleate)



Biodiesel

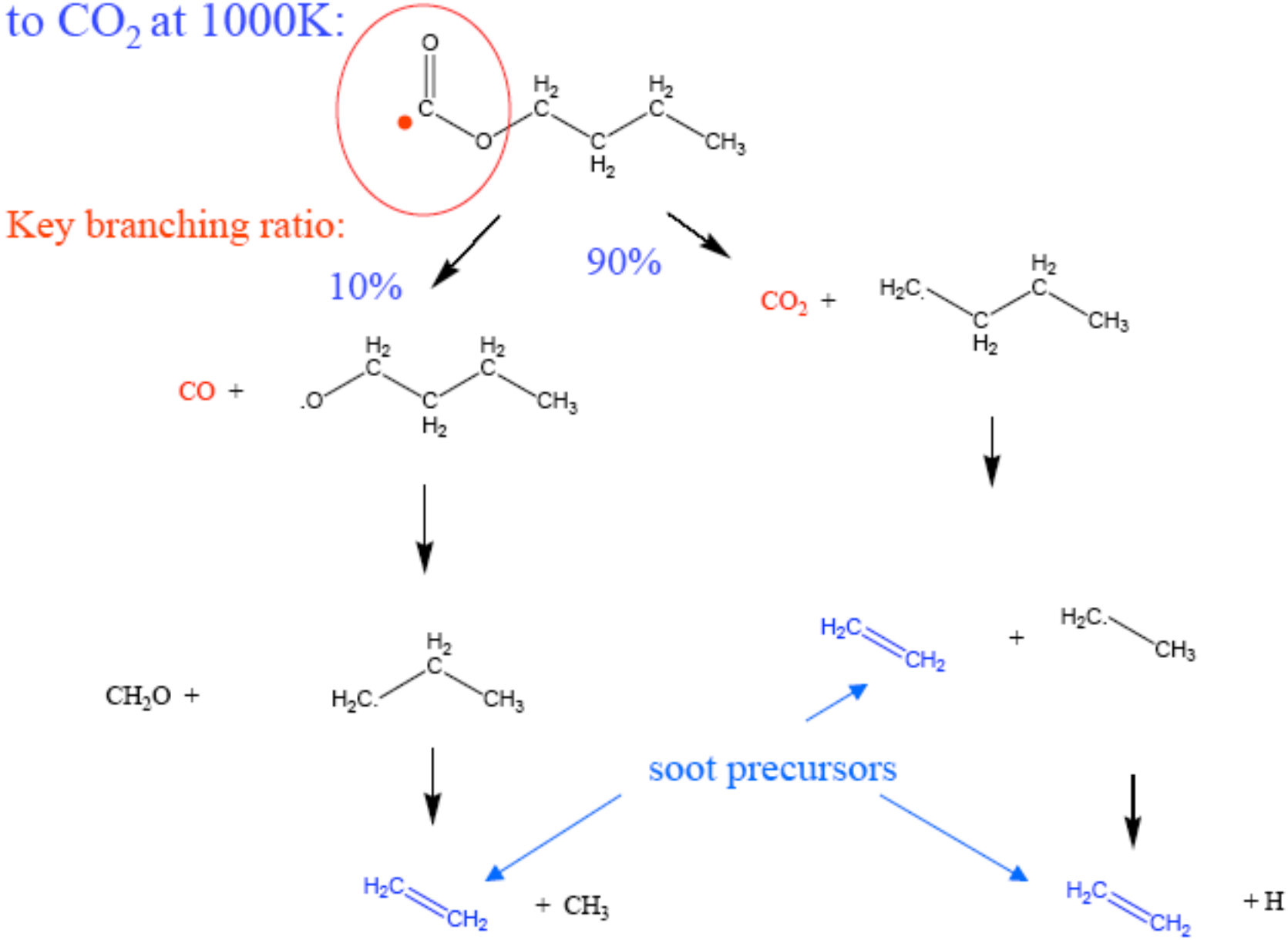
One oxygen atom could be wasted

DMC (dimethylcarbonate) has ester structure



⇒study it, because it is a small, simpler molecule than the large DBM or biodiesel fuels and some experimental data was available

Based on new rates, 90% of key ester structure in DBM goes to CO_2 at 1000K:

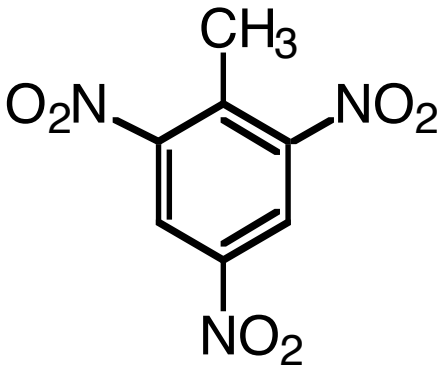


Molecular structure of oxygenated fuel additive determines its soot reduction properties

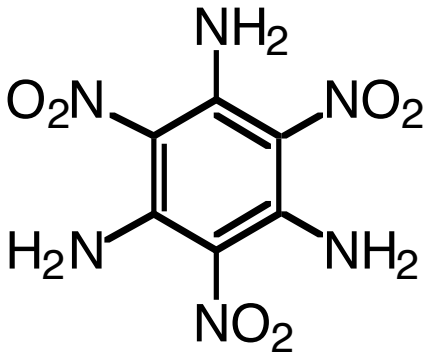
- Variability in soot precursor production observed computationally
- Before modeling approach was used, all oxygenates were believed to be equally effective at soot reduction
- Subsequent engine experiments consistent with model results
- Reaction pathways that lead to early CO_2 production “waste” available oxygen atoms in the oxygenate
- Same approach provided sooting estimates for oil sands fuel
- All analysis based on single-component “diesel fuel” surrogate
- Need for more thorough, multicomponent diesel simulations
- Opportunities for designing optimal oxygenated additives

Soot production in incineration of munitions can be described chemically in terms that are consistent with diesel combustion production of soot

TNT

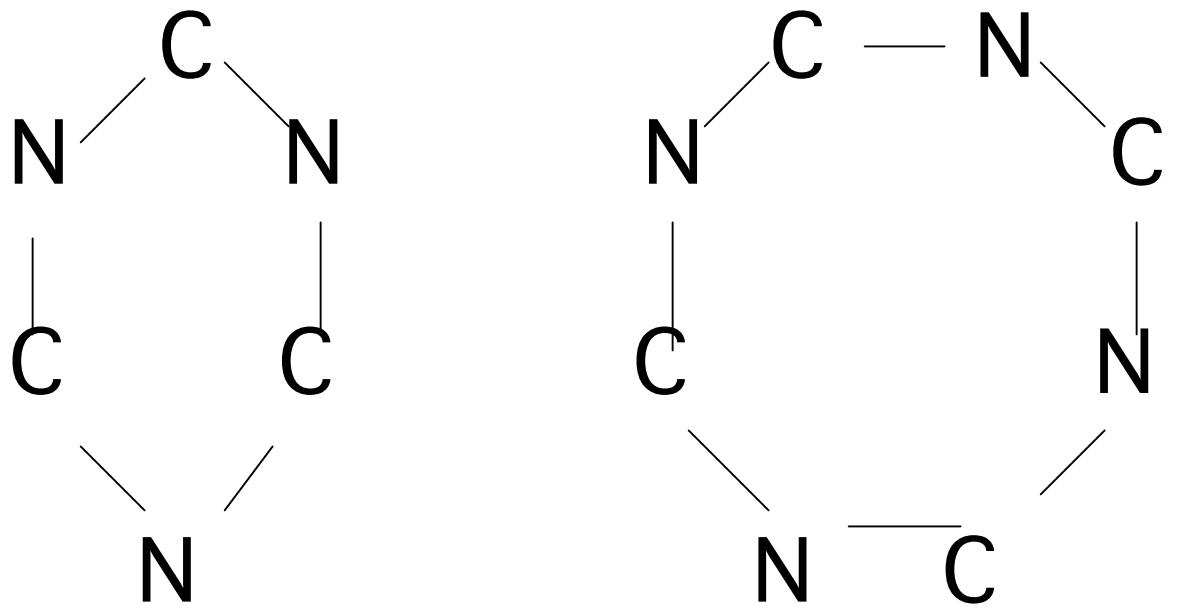


TATB



Presence of aromatic rings indicates explosive will lead to soot.

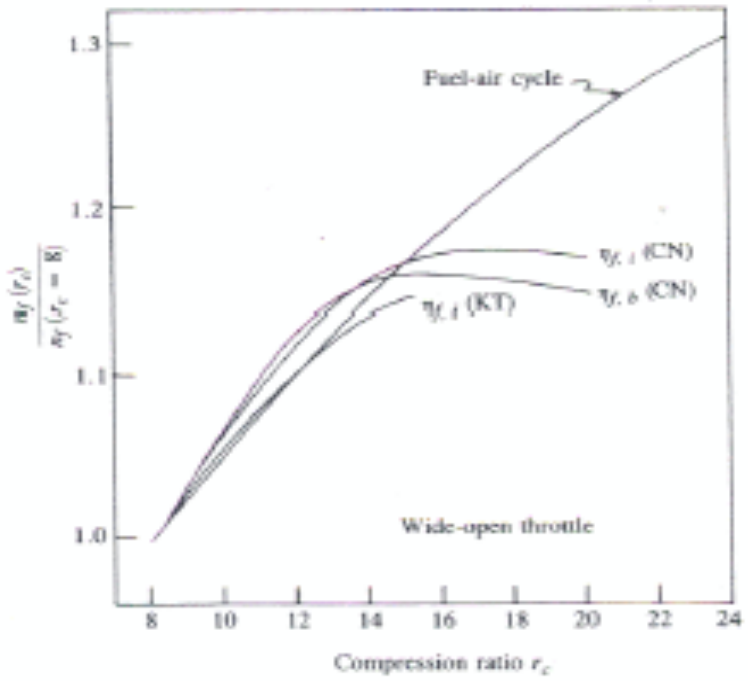
RDX and HMX are based on non-aromatic rings



Note the absence of any C - C bonds or aromatic rings, and these explosives do not produce soot

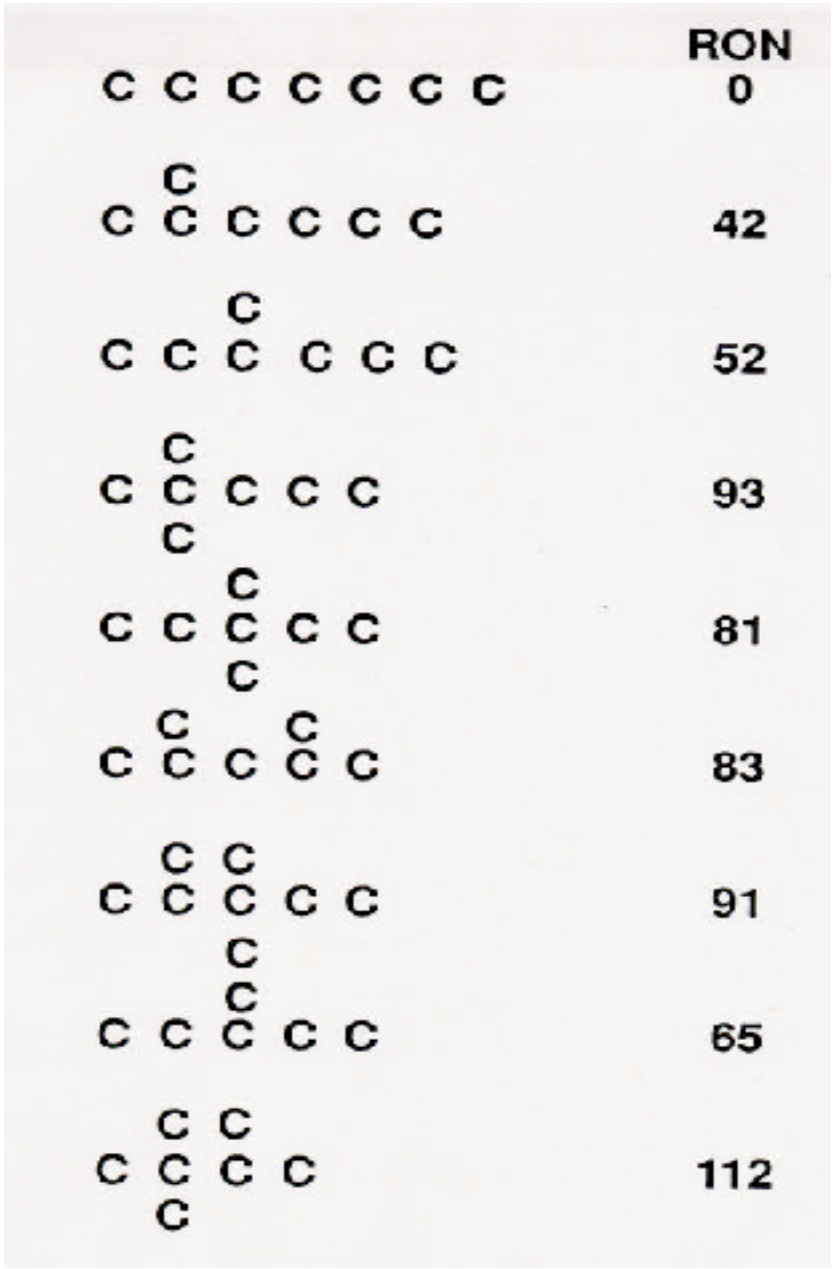
SI engine efficiency increases with compression ratio

- curve of efficiency vs. compression ratio



But onset of engine knock limits compression ratio

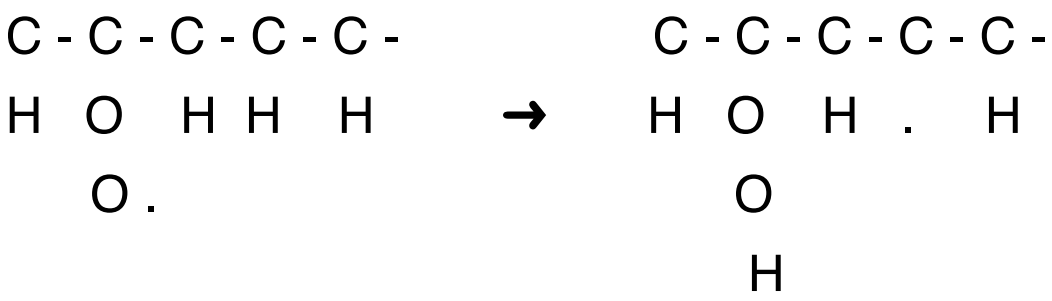
Knock tendency is measured by octane number, which is found to be a strong function of fuel molecule size and structure



We have learned a lot about knock kinetics

- Octane numbers of individual hydrocarbon molecules
  - placed 75 years of observations on a solid theoretical base
- Role of low temperature reaction pathways
  - identification of specific reactions that have the greatest influence
- Mode of action of antiknocks from TEL to MTBE
- But most quantitative details are still poorly understood

Main reaction pathway is internal transfer of H



This chain branching reaction sequence has been studied experimentally and theoretically only for the ethyl peroxy radical

Major improvements in efficiency might be possible with better knowledge of intermediate temperature chain branching kinetic processes

Better antiknock additives could improve efficiencies by delaying onset of engine knock

The HCCI engine is a truly new engine concept

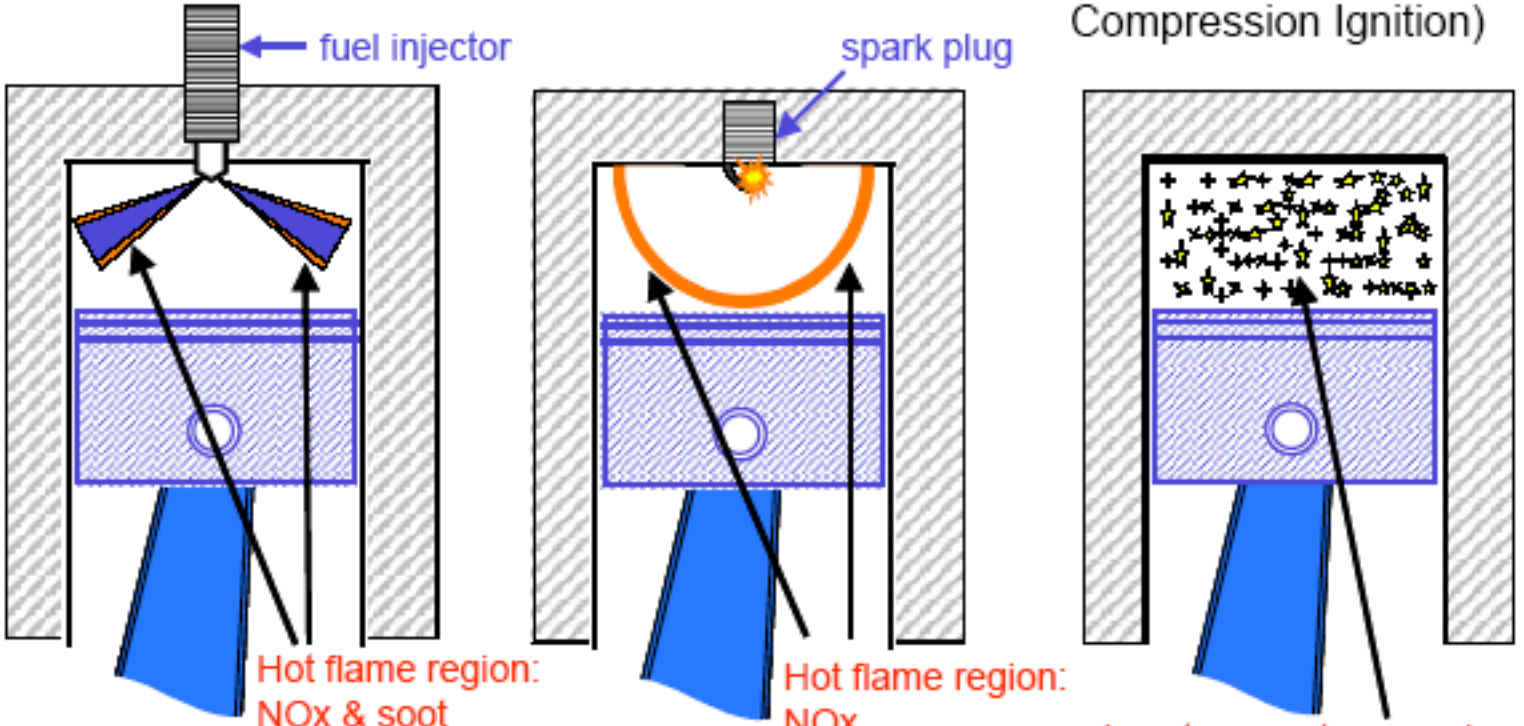
- Premixed gaseous mixture of fuel and air (similar to SI)
- Compression ignition (similar to diesel)
  - High compression ratio gives high efficiency
- New feature is overall very fuel-lean combustion
- Product temperatures too low to produce NOx
- Only way to increase load is to increase fuel fraction
- No flame propagation -- nearly homogeneous ignition
  - Too lean to support flame propagation
- Onset of ignition kinetically controlled, difficult to vary
- Only significant emission is unburned hydrocarbons from wall layers
  - Avoids NOx / UHC tradeoff

What Is HCCI?

Diesel Engine
(compression ignition)

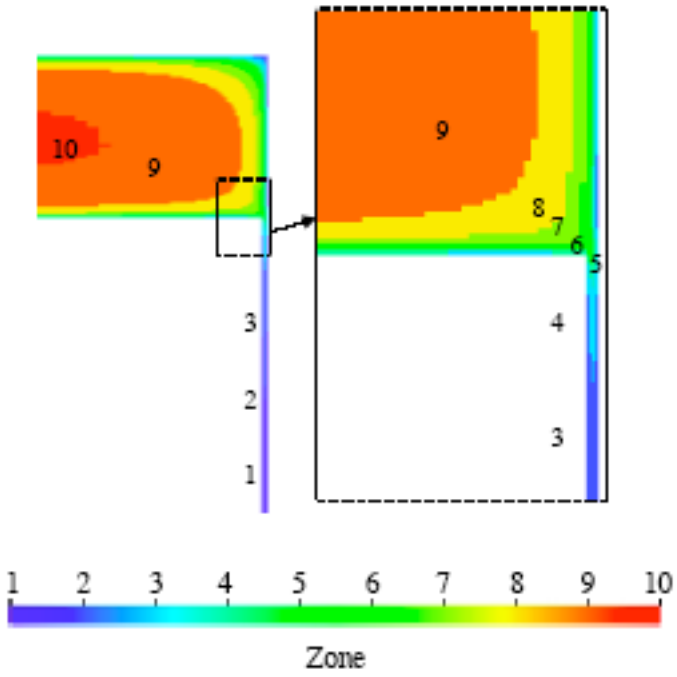
Gasoline Engine
(spark-ignition)

HCCI Engine
(Homogeneous Charge Compression Ignition)



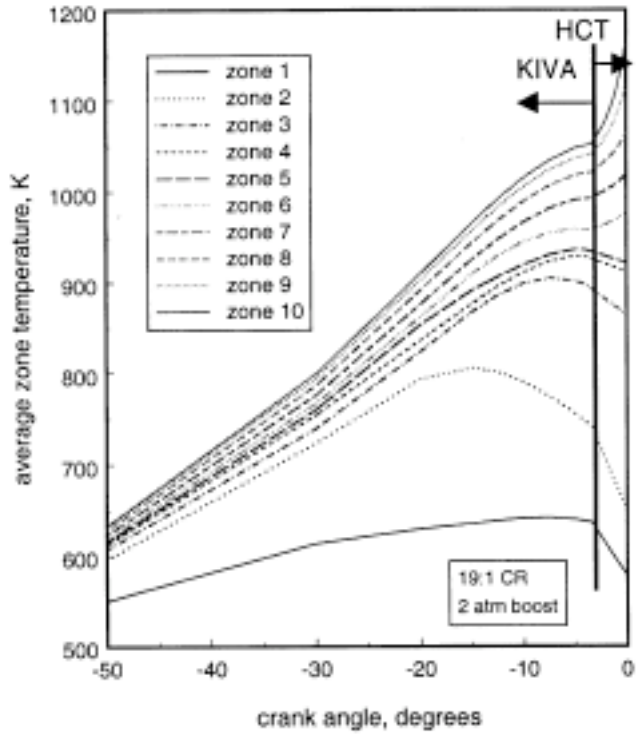
Drawing from Gerald Coleman, Caterpillar Inc.

A multizone simulation of HCCI combustion identifies regions of similar reaction histories and shows the sources of unburned fuel

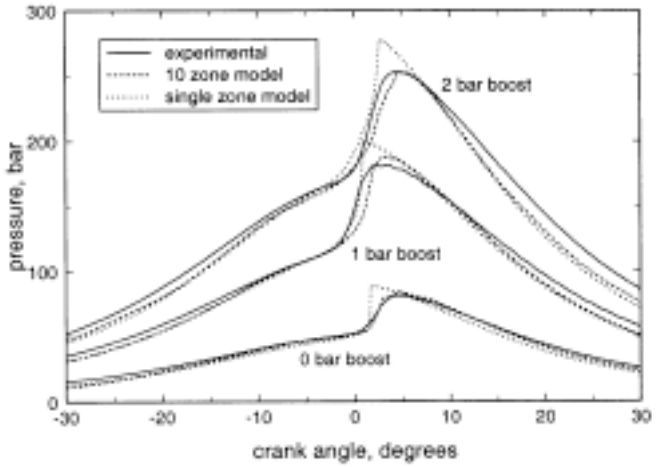


Quenching of reaction by heat transfer is the major source of incomplete reaction

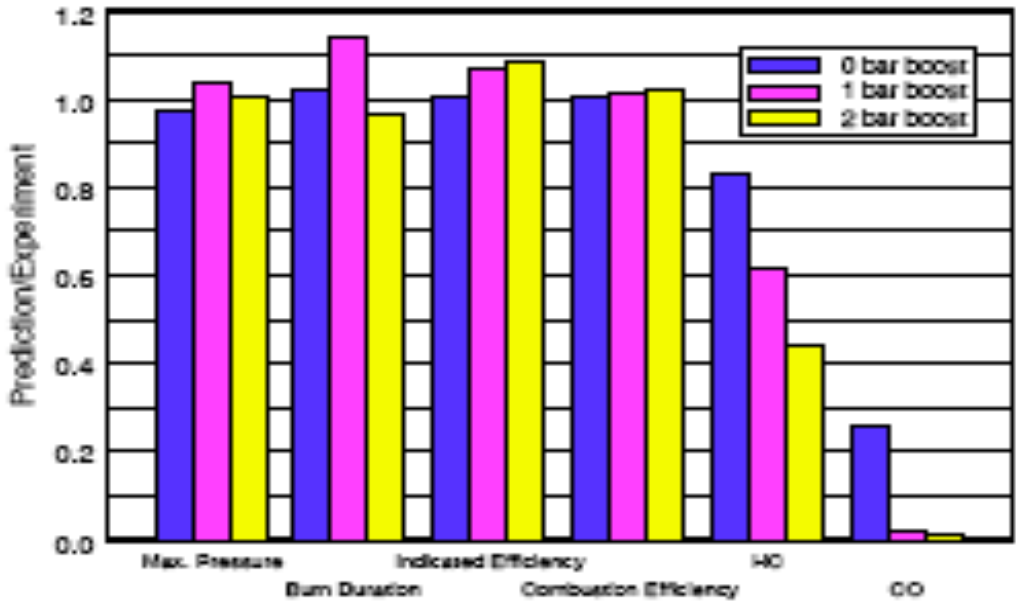
A small number of zones burn incompletely or not at all and produce unburned hydrocarbon emissions



A fairly simple 10 zone chemical model reproduces most of the features of the engine combustion



Most measured parameters are described well, but major emissions are not described properly



Main research needs for HCCI combustion

- Low temperature unburned hydrocarbon catalyst
  - For lean mixtures, product temperature is unusually low
- An effective control system for ignition timing
  - Bowman group is a leader in this area
- A viable alternative to current design strategies of auto industry
  - HCCI over full range of speeds and loads is not best use of technology
  - Perhaps use HCCI as part of hybrid system
  - HCCI ideal for some applications with constant speed and load

Technologies surveyed or excerpted

- Oil sands
- Surrogates for practical transportation fuels
- Diesel engines
- Laser sheet experiments to elucidate physical processes
- Diesel soot production
- Oxygenated diesel fuel additives for soot reduction
- Engine knock
- HCCI combustion principles

Closing observations

- Combustion is major source of CO_2 emissions, so increased combustion efficiency provides huge opportunities for reduced emissions
- Many potential strategies for increased efficiency are being examined but further research is needed
- Past and current examples show that science-based improvements in combustion technologies can be very productive
- Role of computer simulations in modern combustion research has become extremely important
- Industry seems very willing to embrace technical advances from new experimental and computational techniques

Acknowledgments

Thanks to William Pitz at LLNL and John Dec and Mark Musculus at Sandia Livermore for valuable input and slides for this presentation.

This work was carried out under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.