SAND2016-6909C

Sooting tendencies of diesels, jet fuels, and their surrogate components

Dhrubajyoti D Das, William J Cannella, Charles S McEnally,
Charles J Mueller, Lisa D Pfefferle

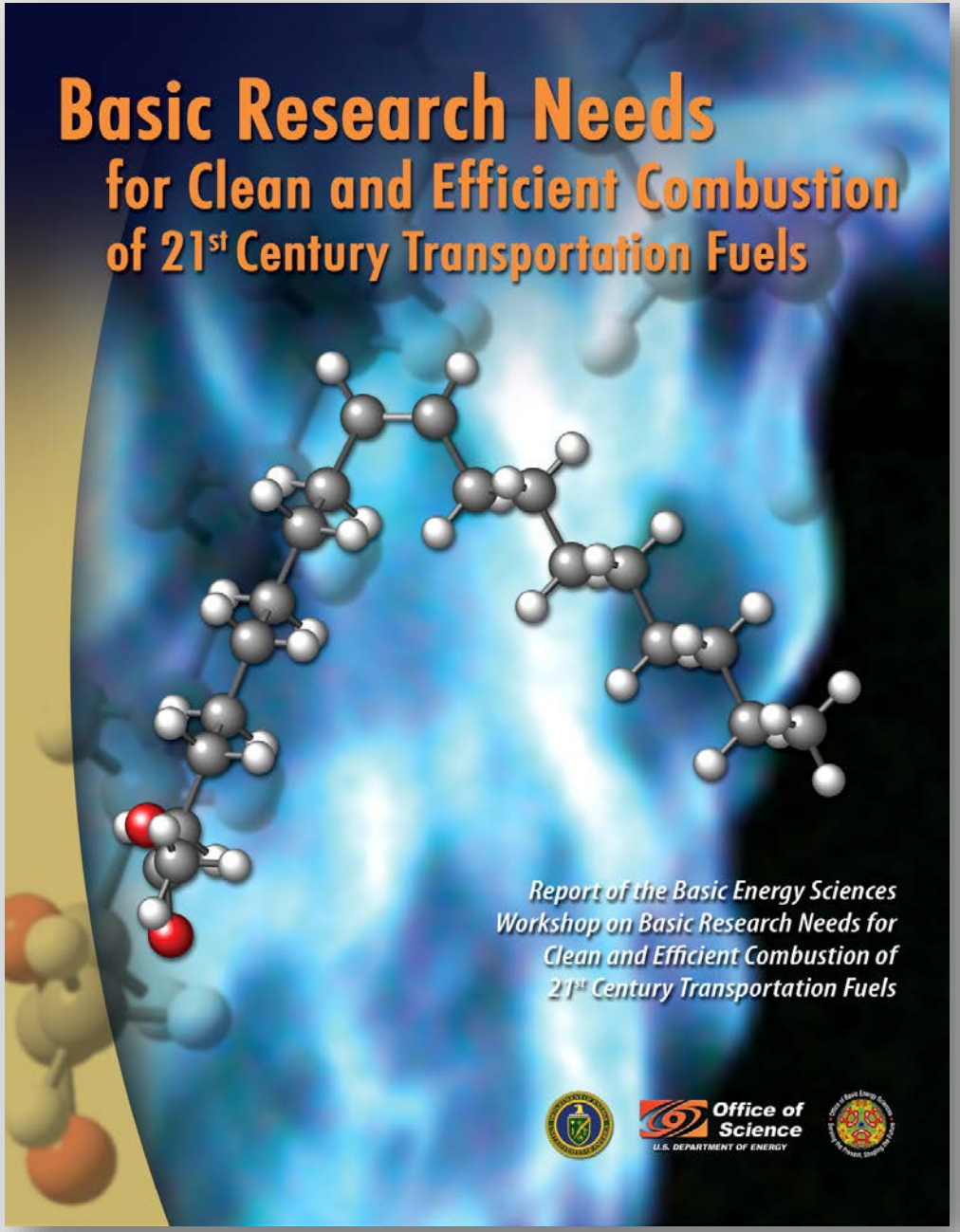
Yale

Sandia National Laboratories

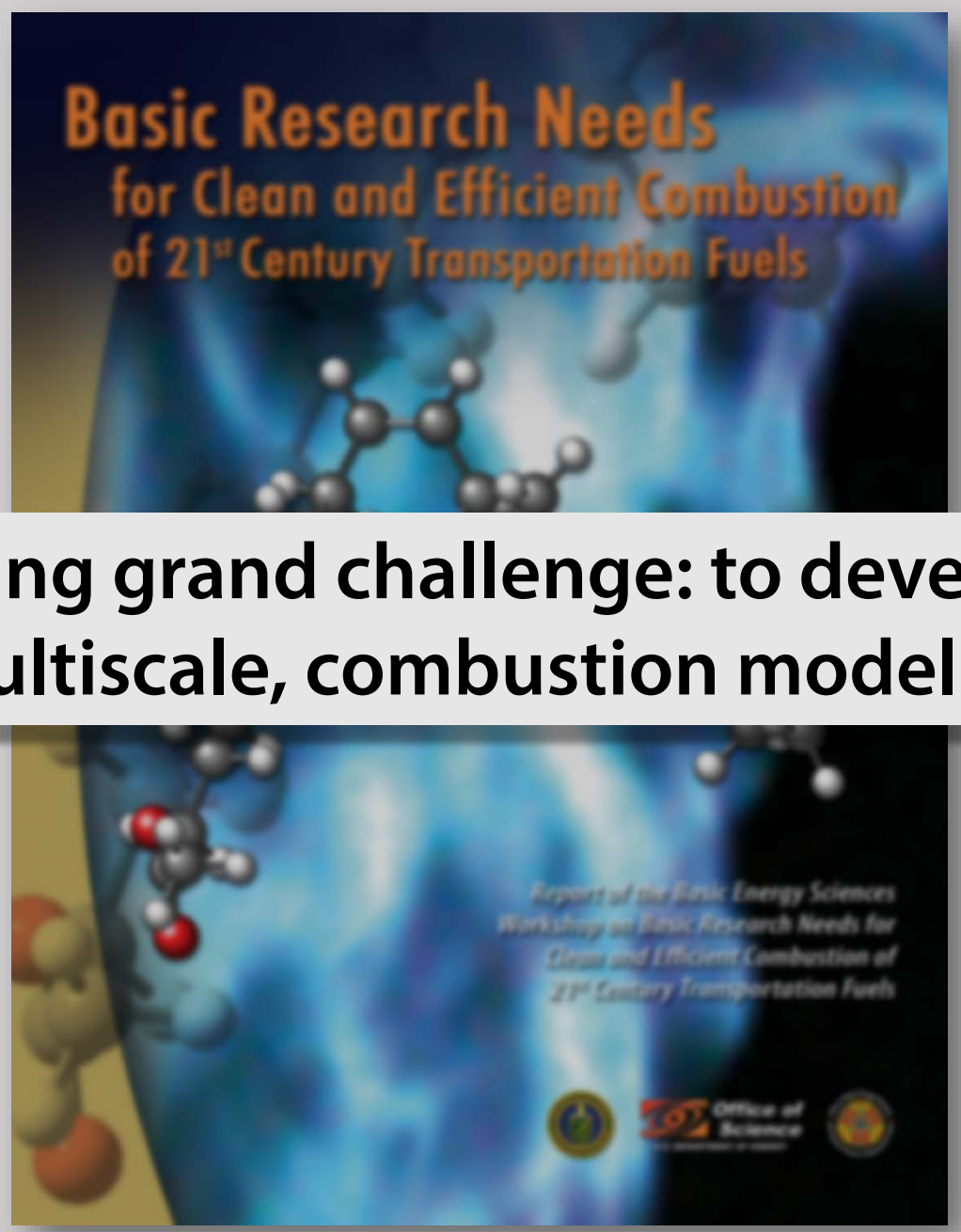
Chevron

Supported by the National Science Foundation and the United States Department of Energy

Introduction



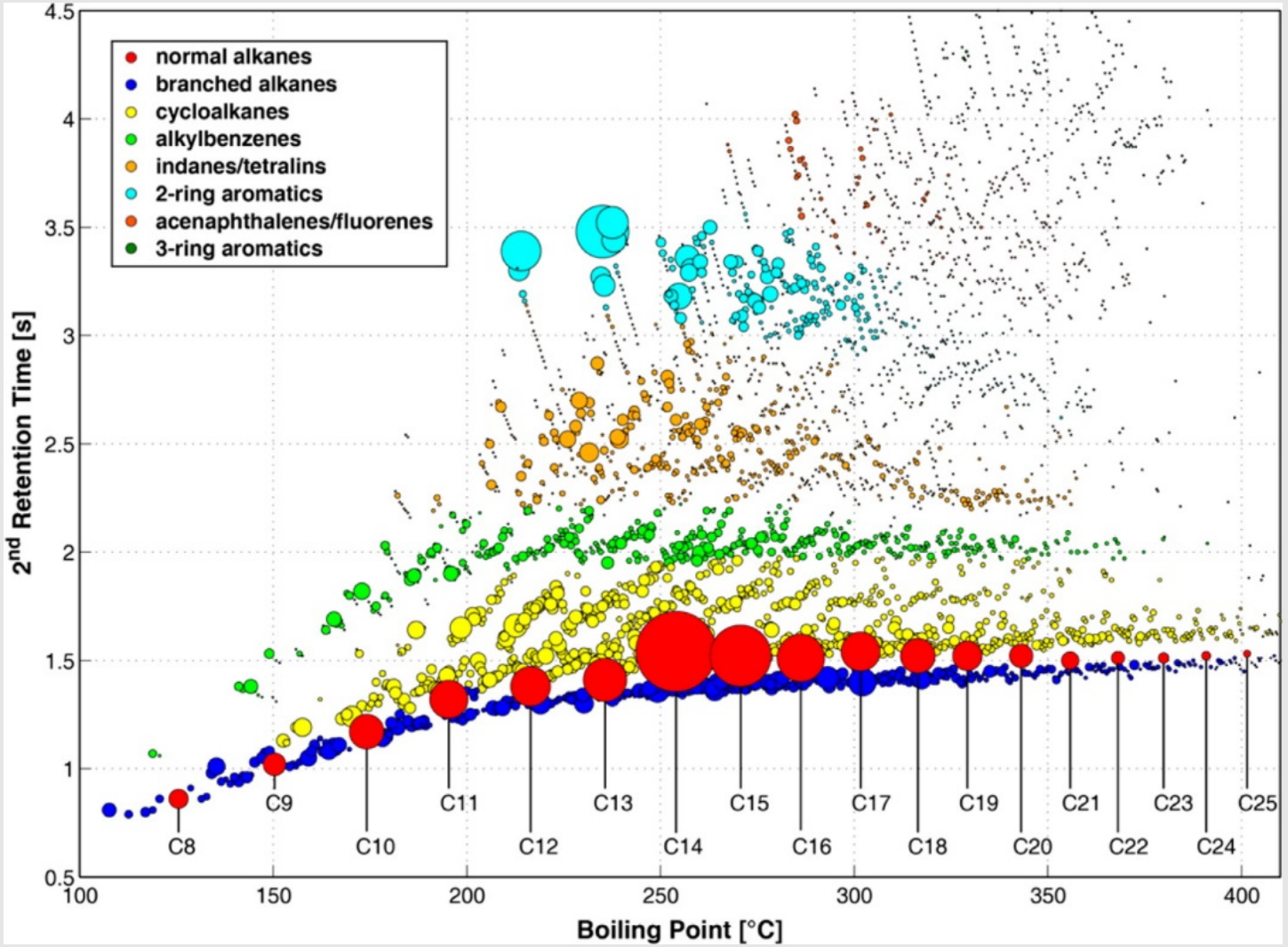
sc.doe.gov/bes/reports/files/CTF_rpt.pdf



One overarching grand challenge: to develop validated, predictive, multiscale, combustion modeling capability

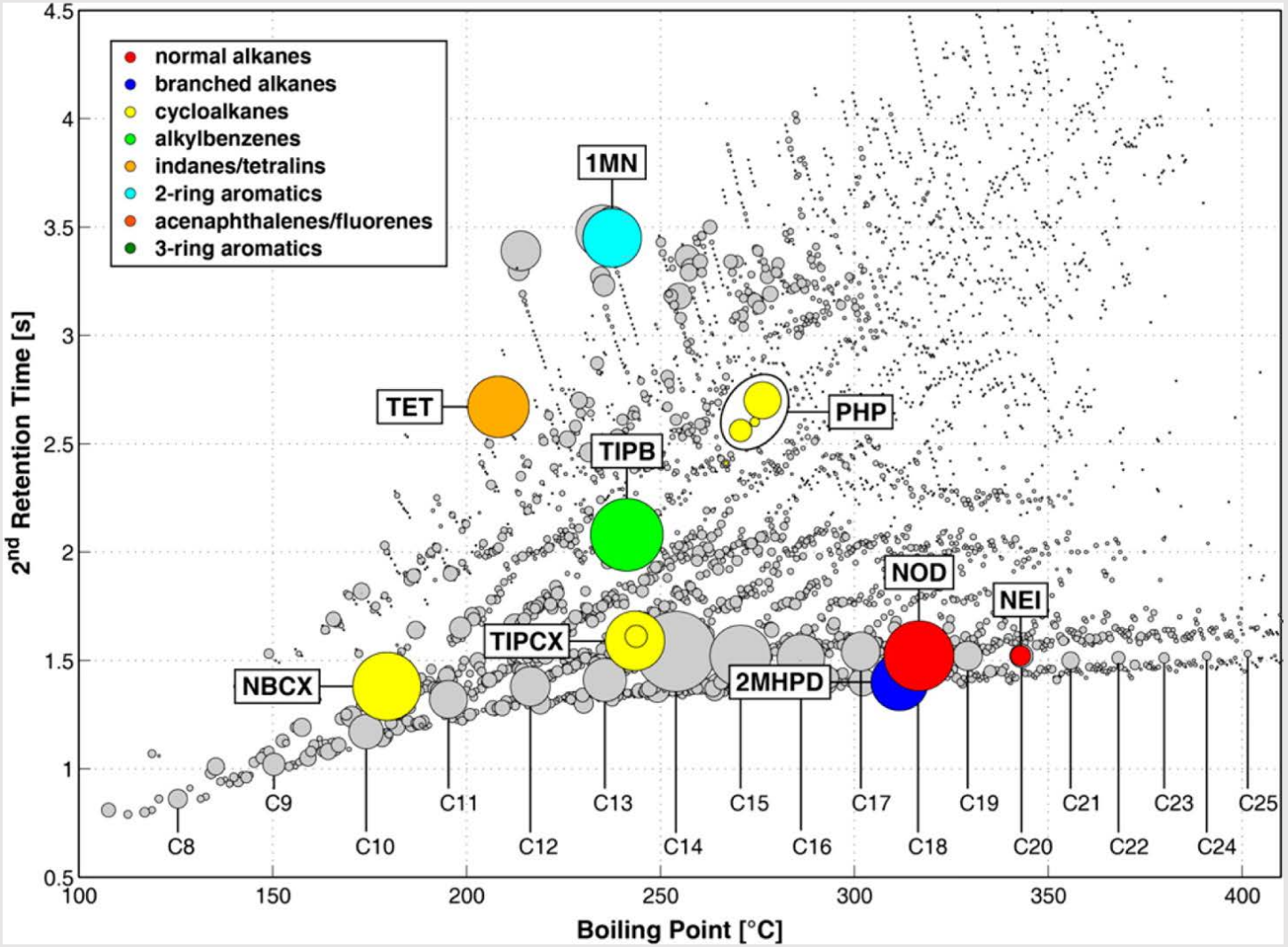
sc.doe.gov/bes/reports/files/CTF_rpt.pdf

Need for studying more complex fuels



C. J. Mueller et al. *Energy & Fuels*, 30 (2016), 1445–61

Need for studying more complex fuels



C. J. Mueller et al. *Energy & Fuels*, 30 (2016), 1445–61

Need for studying more complex fuels

Issues

1. Low volatility, difficult to vaporize
2. Highly sooting, causes diagnostic issues
3. Spray flames, complex fluid mechanics

Doped methane flames

1. Easy to introduce low volality fuels
2. Methane is simple, well-studied
3. Effective test of rxn. mech. for soot

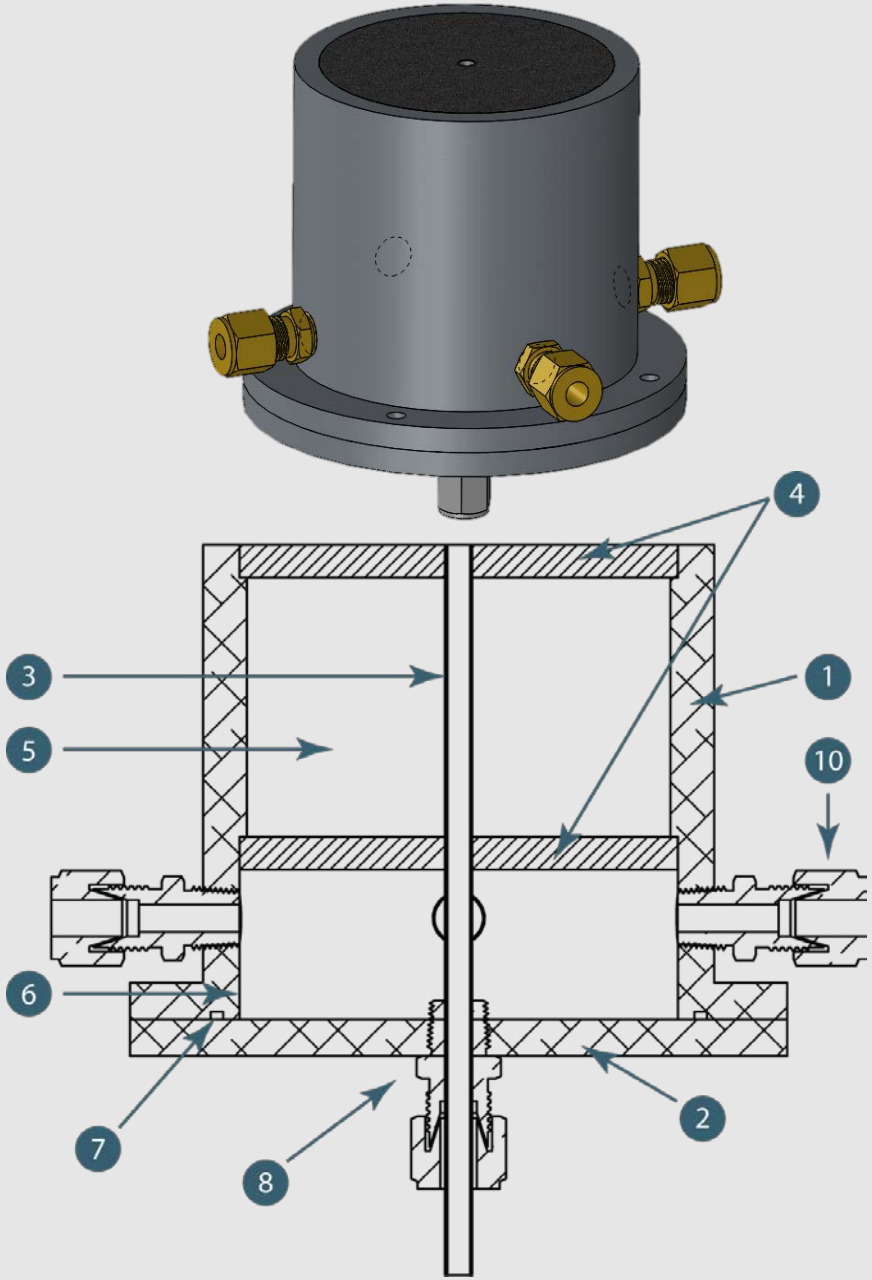
Dopant	0.5% by mass
CH_4	58% by mass
N_2	Balance
Total	19.2 g/hr (~400 cc/min)

Fuel **Air**

Experimental Approach

Yale Coflow Burner

- Standardized at 2nd ISF Workshop
- CAD files available for download/machining



Yale Coflow Burner

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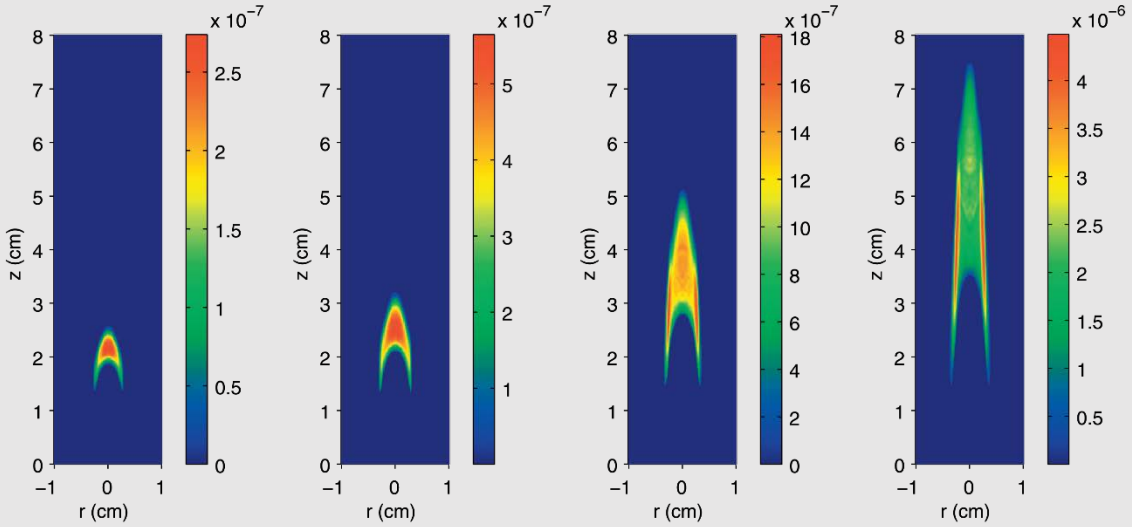
Soot color ratio pyrometry

Soot and thin-filament pyrometry using a color digital camera

Peter B. Kuhn, Bin Ma, Blair C. Connelly, Mitchell D. Smooke, Marshall B. Long *



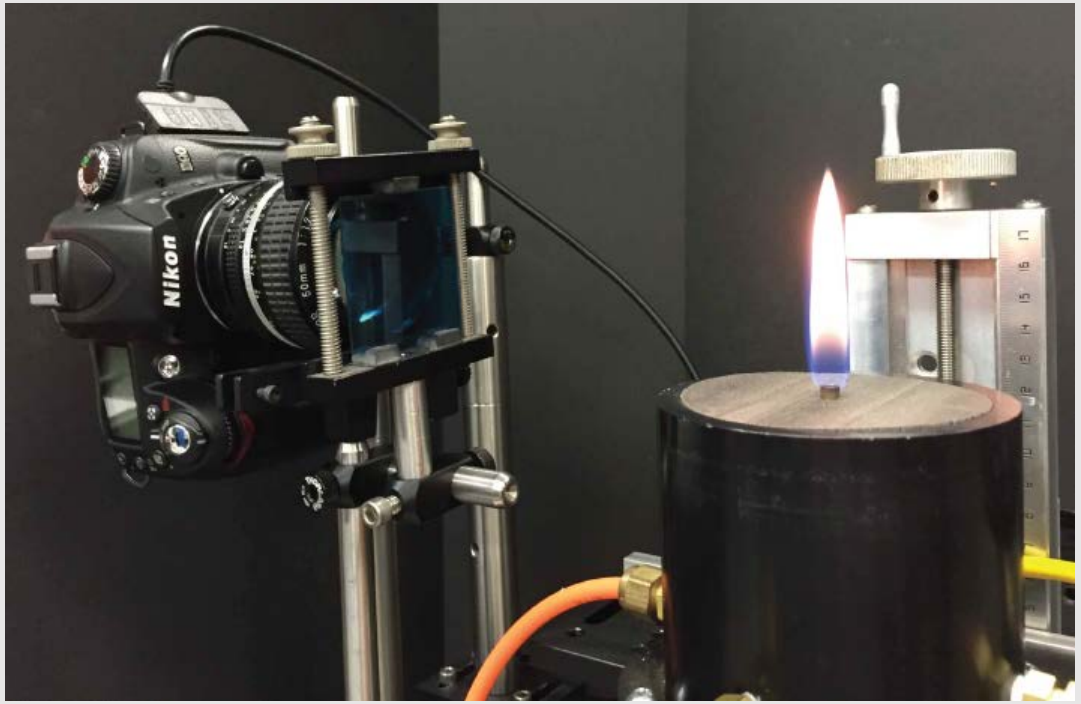
Kuhn et al., Proc. Comb. Inst. 33 (2011) 743–750

Yale Coflow Burner

- Standardized at 2nd ISF Workshop
- CAD files available for download/machining

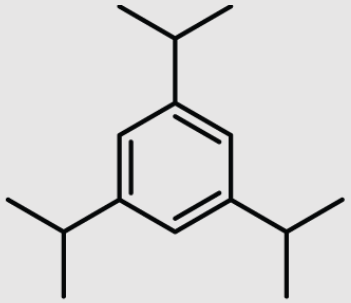
Soot color ratio pyrometry

- Nikon D90 camera for image capture
- Line-of-sight inversion with Gaussian basis set expansions approach (BASEX)[1]
- Soot emissivity modeled as $\varepsilon(\lambda) = \lambda^{-1.38}$
- Type-S thermocouple for absolute light calibration

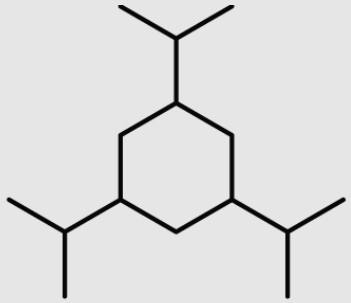


[1] V. Dribinski et al. *Rev. Sci. Instru.*, 73 (2002), 2634–42

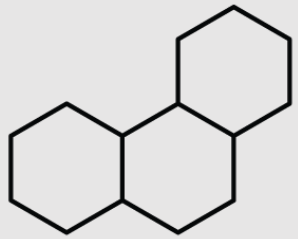
Compounds and fuels studied



1,3,5-triisopropylbenzene
(TIPB)



1,3,5-triisopropylcyclohexane
(TIPCX)



perhydrophenanthrene
(PHP)

D.D. Das, W.J. Cannella, C.S. McEnally, C.J. Mueller, and L.D. Pfefferle, "Two-dimensional soot volume fraction measurements in flames doped with large hydrocarbons," *Proceedings of the Combustion Institute*, (in press).

Compounds and fuels studied

- Two reference diesels
  - CFA, FD9A
- Four reference jet fuels
  - POSF 4658, 10264, 10289, 10325
- Four surrogate diesels [1]
  - SDV0A, SDV0B, SDV1, SDV2
- Five surrogate jet fuels
  - AACHEN [2], DREXEL [3], PRINCETON [4], PENN STATE [5], UTAH [6]

- 27 pure compounds
  - 10 alkanes, 10 aromatics, 5 cyclic alkanes, 2 cyclic aromatics
  - Size range C_6 - C_{20}
  - M.W. range 78 - 282 g/mol
  - B.P. range 68 °C - 315 °C

1. C. Mueller et al., *Energy & Fuels* 30 (2016) 1445-61
2. S. Honnet et al., *Proc. Comb. Inst.* 32 (2009) 85-92
3. A. Agosta et al., *Expt. Therm. Fl. Sci.* 28 (2004) 701-708
4. S. Dooley et al., *Comb. and Flame* 159 (2012) 1444-66
5. A. Mensch et al., *Comb. and Flame* 157 (2010) 1097-1105
6. A. Violi et al., *Comb. Sci. Tech.* 174 (2002) 399-417

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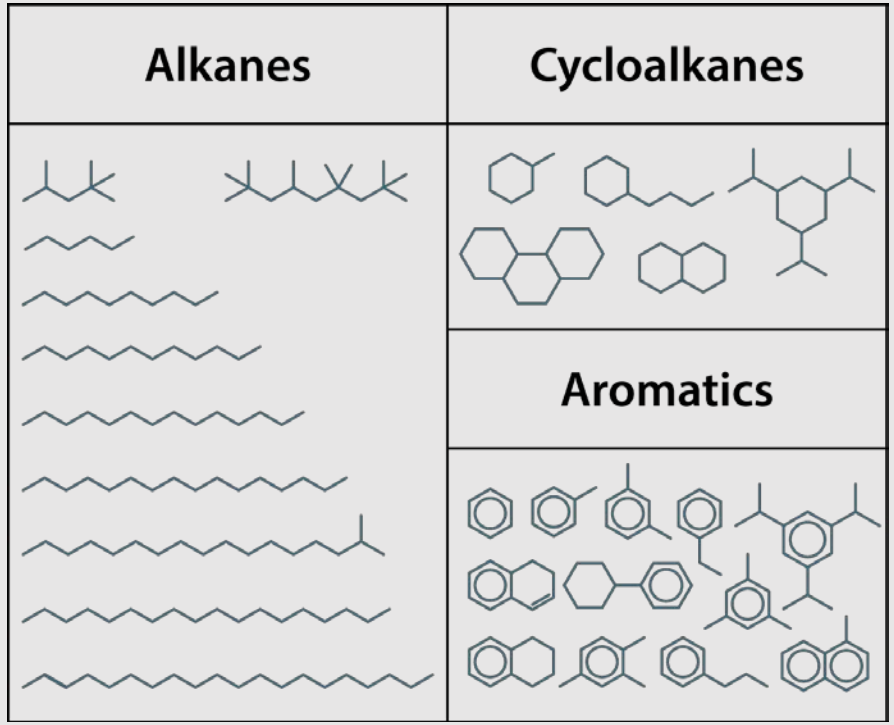

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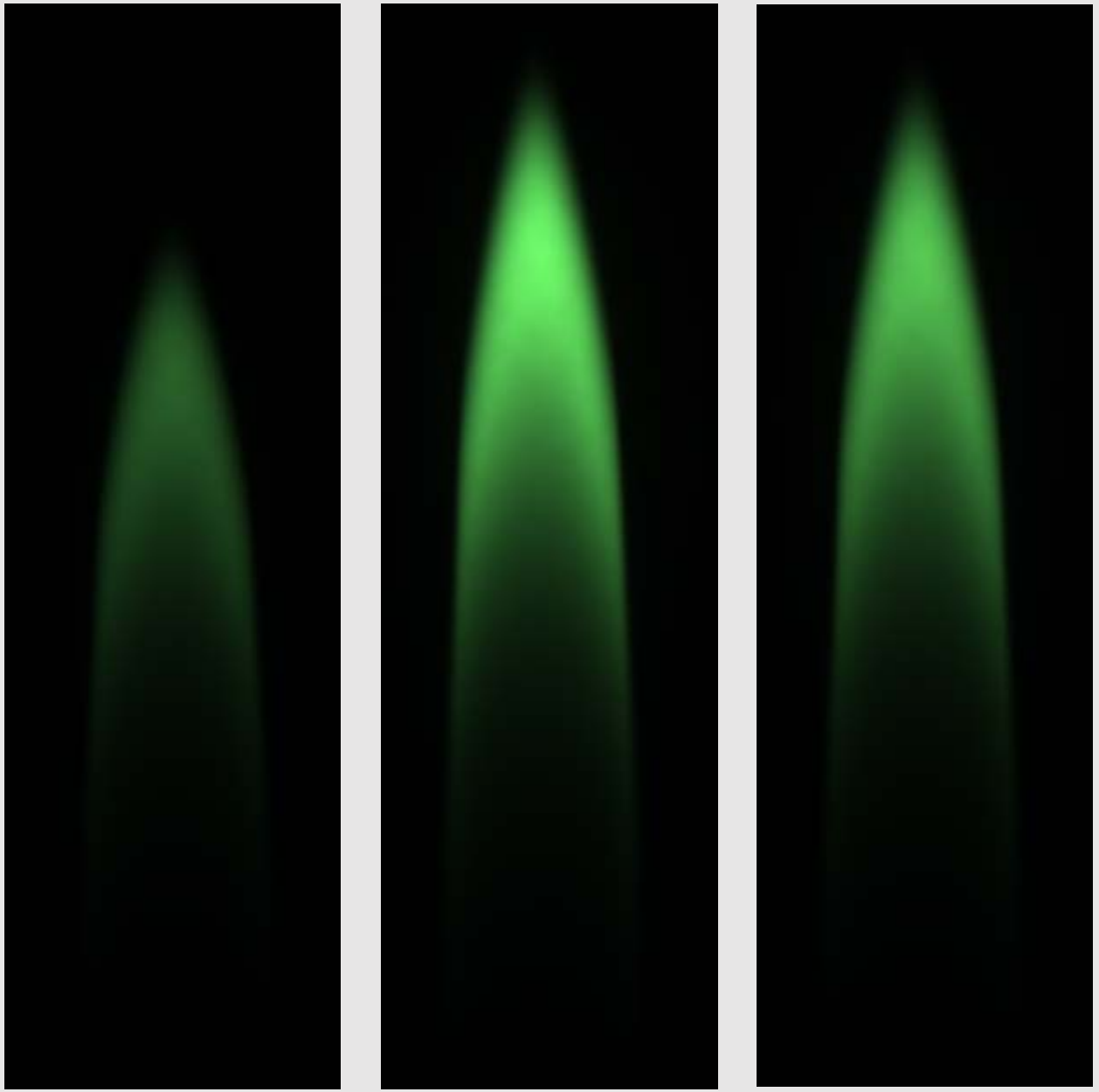
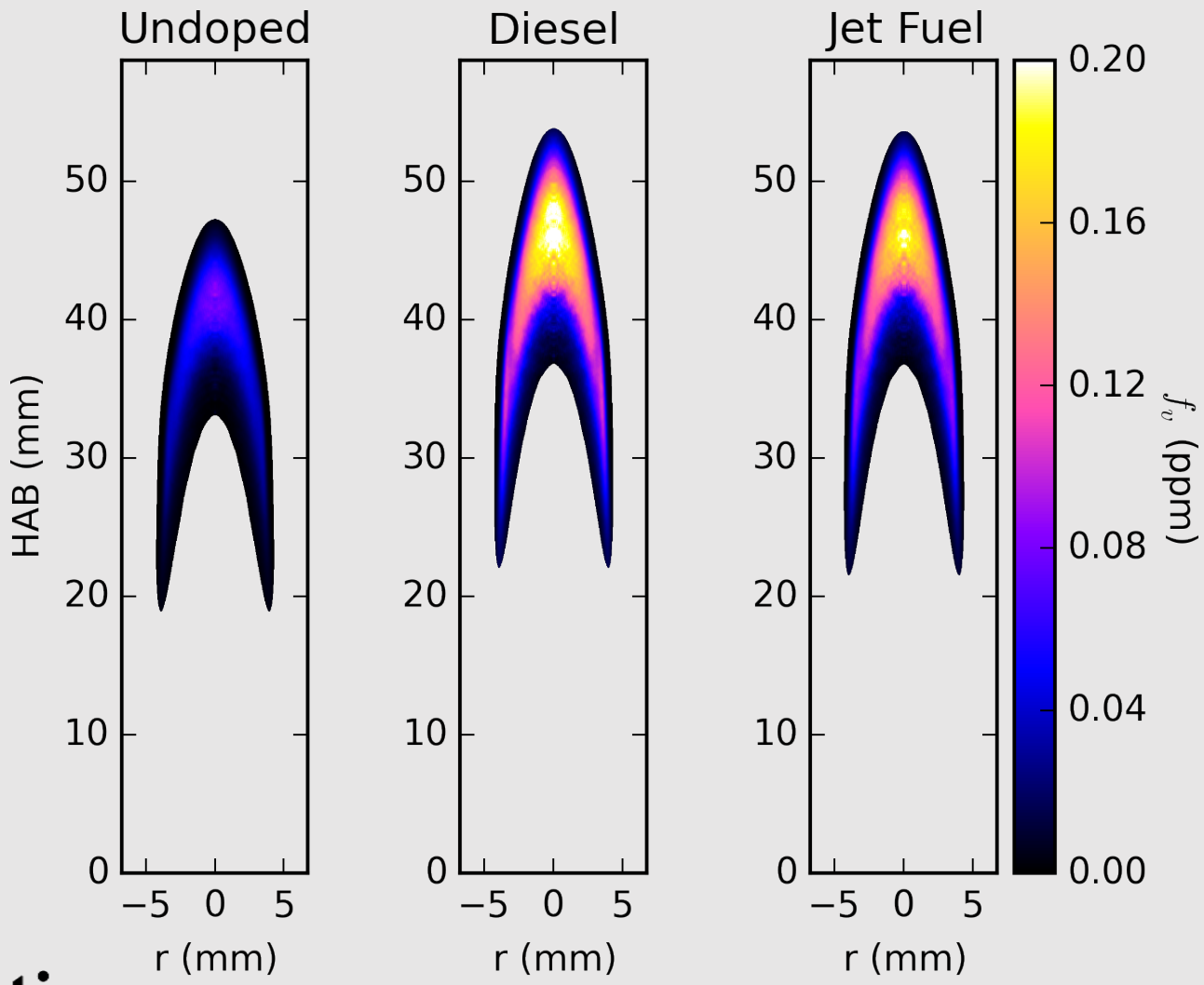
Results

- Undoped methane flame
- Methane flame doped with diesel fuel (CFA)
- Methane flame doped with jet fuel (POSF 4058)



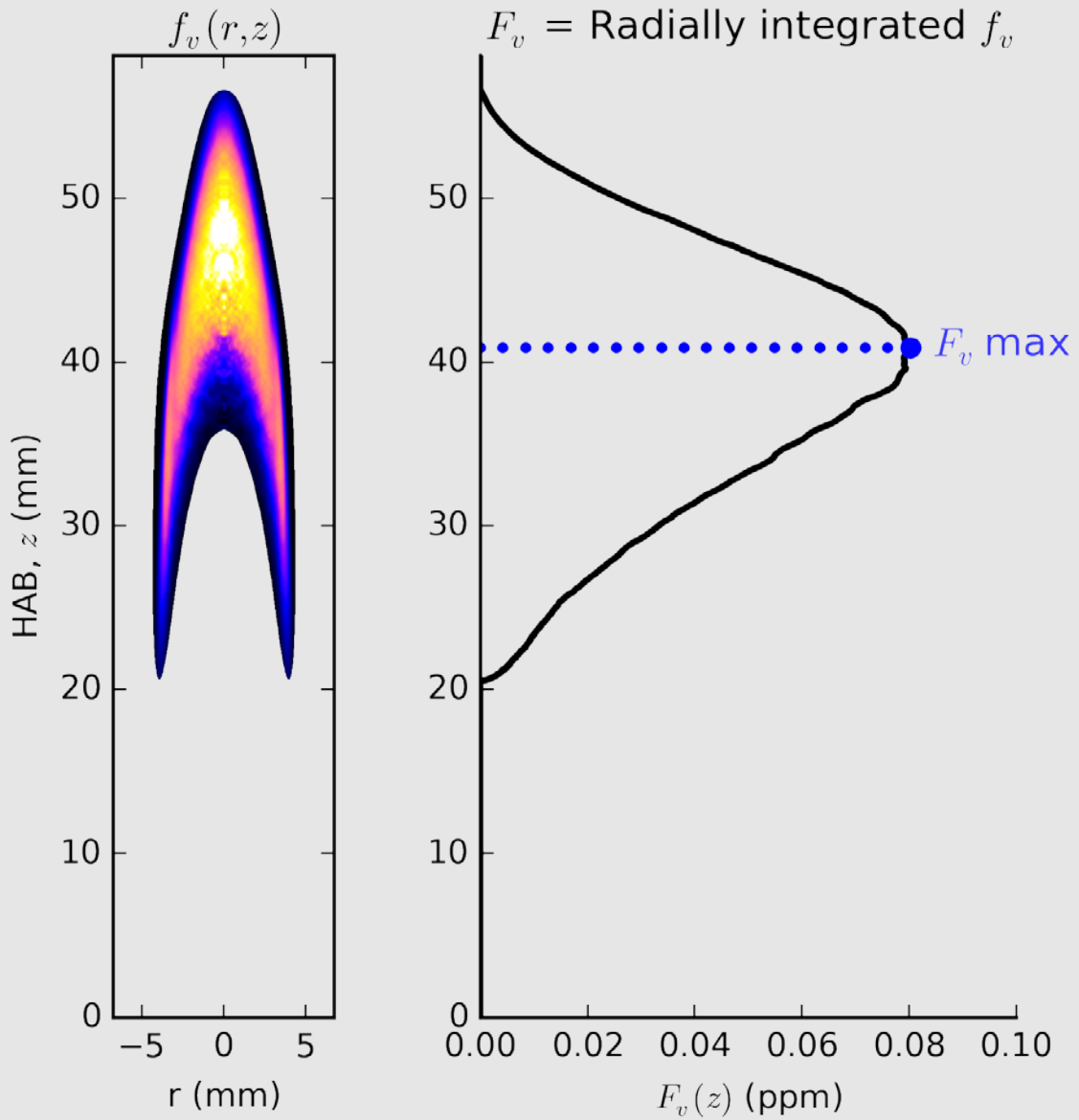
Raw flame image

- Undoped methane flame
- Methane flame doped with diesel fuel (CFA)
- Methane flame doped with jet fuel (POSF 4058)

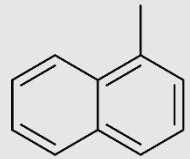


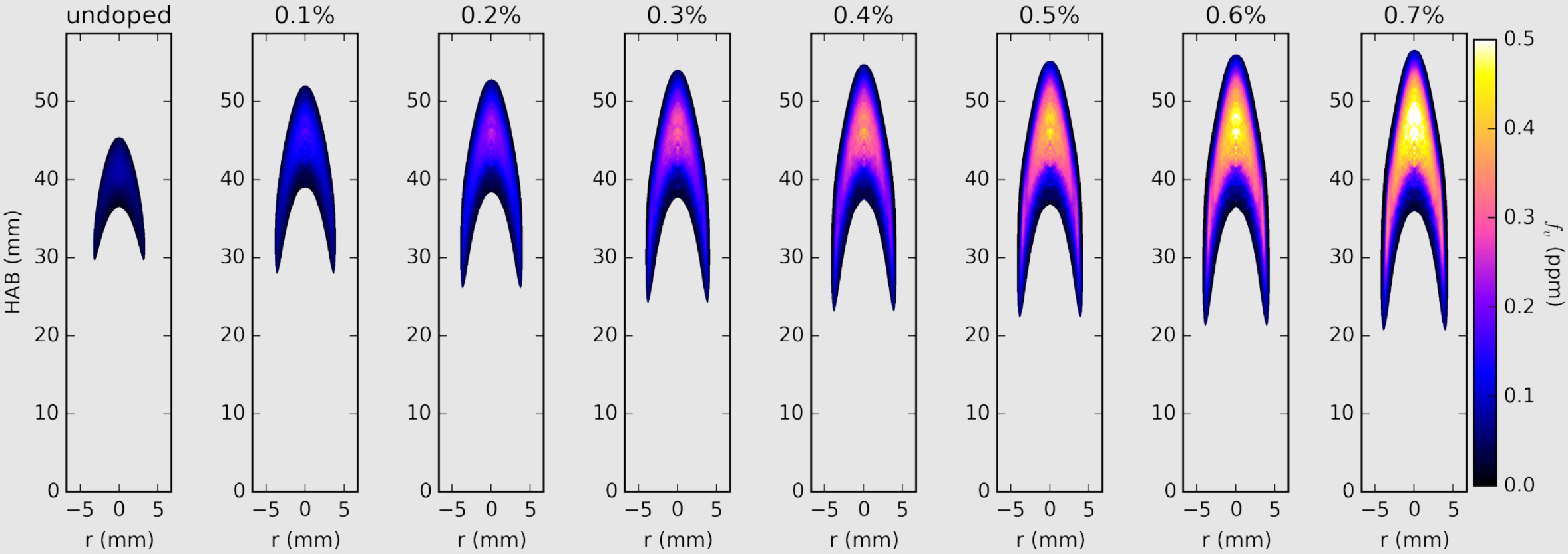
Soot volume fraction

$$F_v(z) = \frac{1}{\pi R^2} \int_0^R 2\pi r f_v(r,z)\, dr$$



- Methane flame doped with 1-methylnaphthalene





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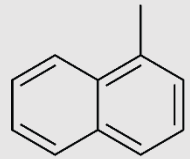
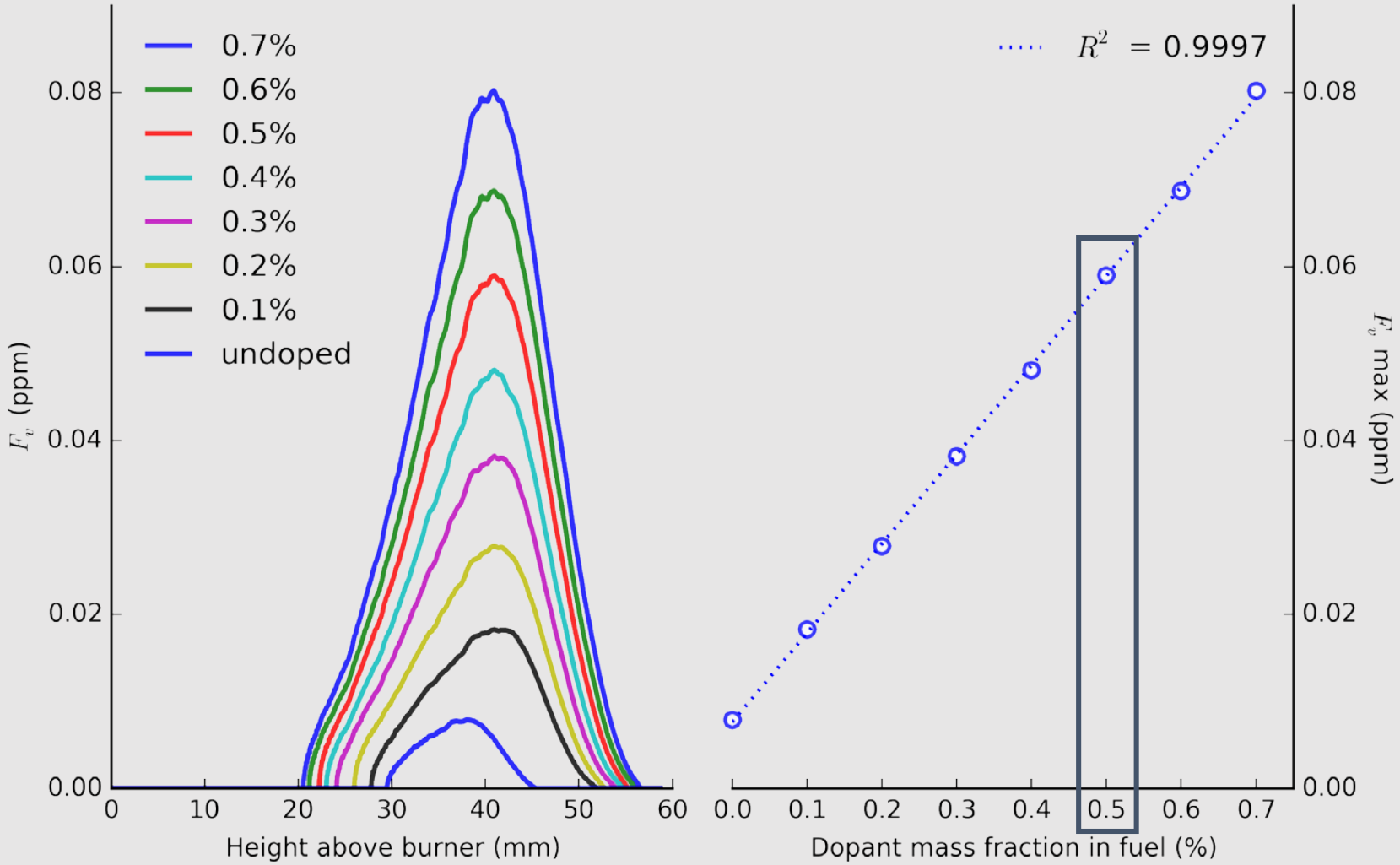


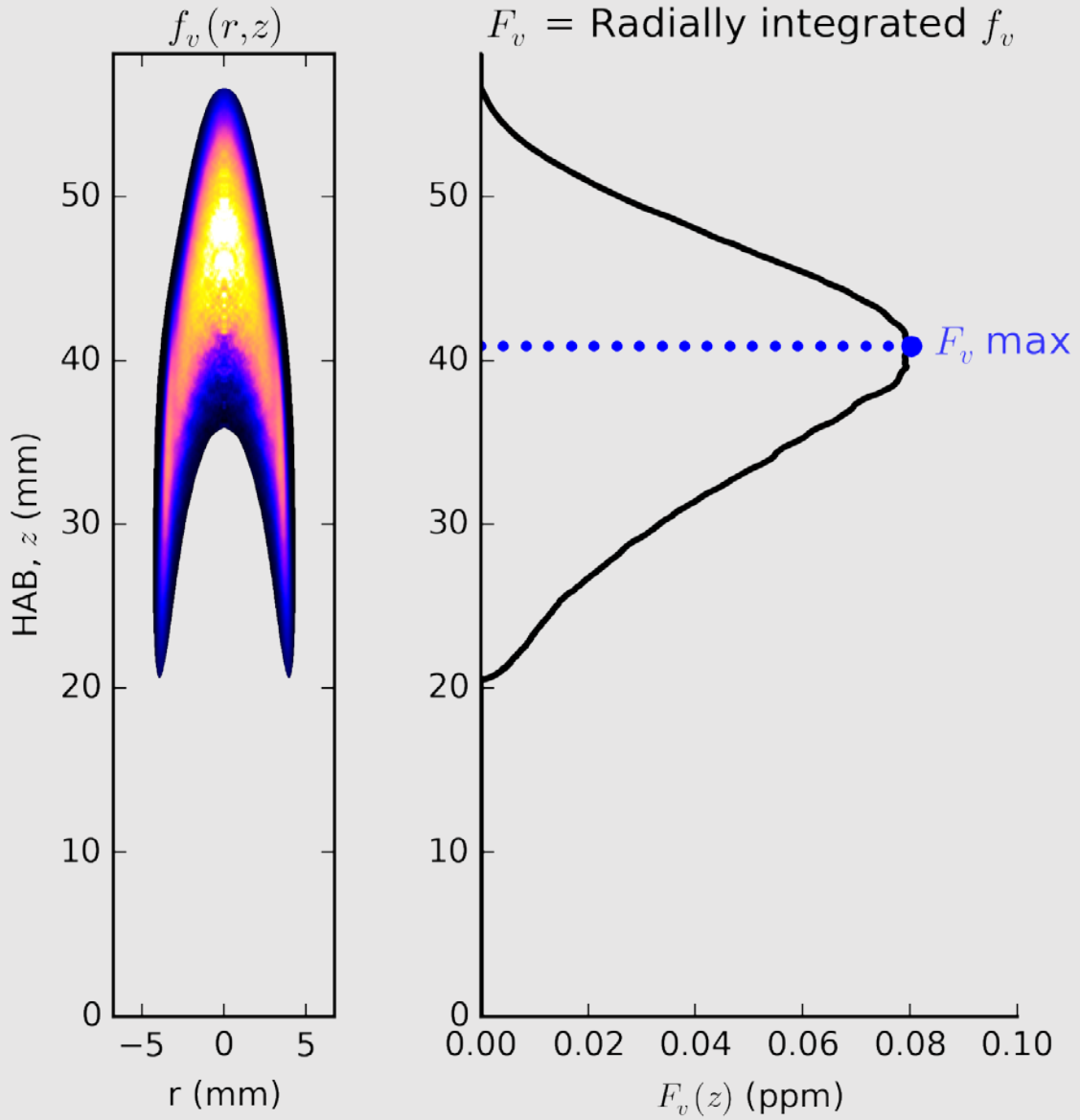


$$F_v(z) = \frac{1}{\pi R^2} \int_0^R 2\pi r f_v(r,z)\, dr$$

$$\text{YSI} = A \times F_v \text{ max} + B$$

0 (hexane)

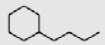
100 (benzene)

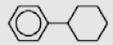
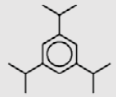
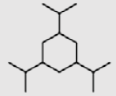
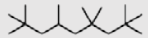
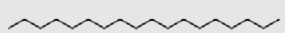


$$\mathrm{YSI} = A \times F_v\ \max + B$$

0 (hexane)

100 (benzene)

IUPAC (Common name)	Formula	YSI[c]	Structure
benzene[a]	C_6H_6	100	
n-hexane[a]	C_6H_{14}	0	
methylbenzene (toluene)	C_7H_8	173	
methylcyclohexane	C_7H_{14}	21	
1,3-dimethylbenzene (*m*-xylene)	C_8H_{10}	193	
ethylbenzene	C_8H_{10}	203	
2,2,4-trimethylpentane (*iso*-octane)	C_8H_{18}	24	
propylbenzene	C_9H_{12}	181	
1,2,4-trimethylbenzene	C_9H_{12}	264	
1,3,5-trimethylbenzene (mesitylene)	C_9H_{12}	243	
1,2-dihydronaphthalene (dialin)	$C_{10}H_{10}$	352	
1,2,3,4-tetrahydronaphthalene (tetralin)	$C_{10}H_{12}$	266	
decahydronaphthalene (decalin)	$C_{10}H_{18}$	47	
n-butylcyclohexane	$C_{10}H_{20}$	18	

IUPAC (Common name)	Formula	YSI[c]	Structure
n-decane	$C_{10}H_{22}$	7	
1-methylnaphthalene	$C_{11}H_{10}$	471	
cyclohexylbenzene	$C_{12}H_{16}$	224	
n-dodecane	$C_{12}H_{26}$	10	
perhydrophenanthrene[b]	$C_{14}H_{24}$	76	
n-tetradecane	$C_{14}H_{30}$	9	
1,3,5-triisopropylbenzene[b]	$C_{15}H_{24}$	246	
1,3,5-triisopropylcyclohexane[b]	$C_{15}H_{30}$	46	
n-hexadecane	$C_{16}H_{34}$	12	
2,2,4,4,6,8,8-heptamethylnonane (*iso*-cetane)	$C_{16}H_{34}$	32	
2-methylheptadecane[d]	$C_{17}H_{36}$	13	
n-octadecane	$C_{18}H_{38}$	20	
n-eicosane	$C_{20}H_{42}$	26	

COMBUSTION AND FLAME 62: 43–60 (1985) 43

The Effects of Molecular Structure on Soot Formation II. Diffusion Flames

D. B. OLSON, J. C. PICKENS, and R. J. GILL

AeroChem Research Laboratories, Inc., P.O. Box 12, Princeton, NJ 08542

Combustion and Flame 157 (2010) 1097–1105

Contents lists available at ScienceDirect

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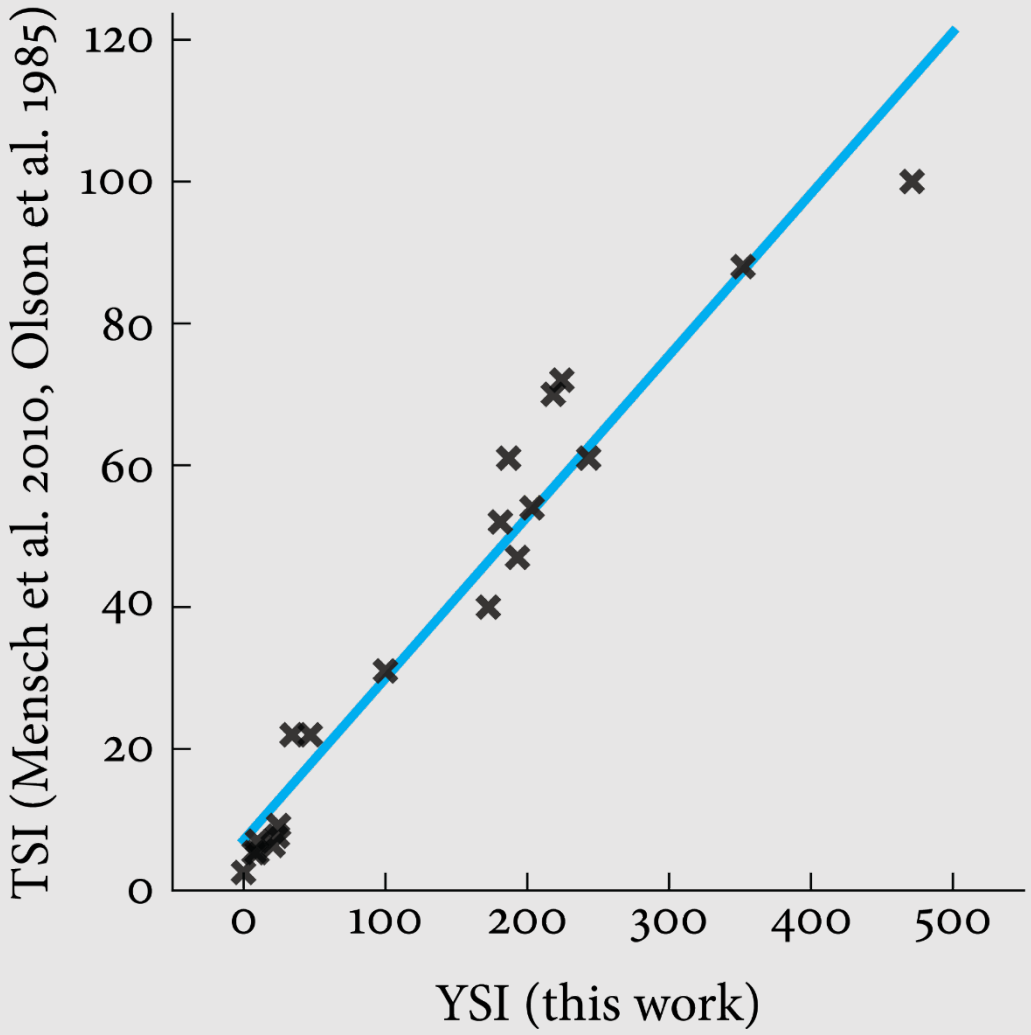
journal homepage: www.elsevier.com/locate/combustflame

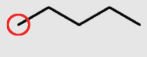
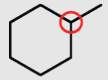
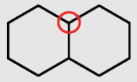
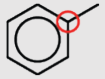
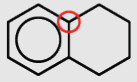
Sooting characteristics of surrogates for jet fuels

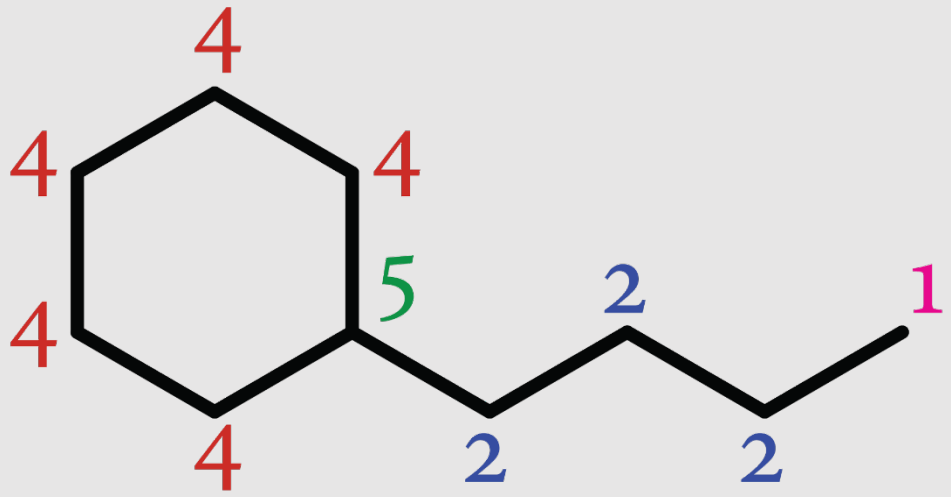
Amy Mensch [a], Robert J. Santoro [a,*], Thomas A. Litzinger [a], S.-Y. Lee [b]

[a] *Department of Mechanical and Nuclear Engineering, and The Propulsion Engineering Research Center, The Pennsylvania State University, University Park, PA 16802, United States*
[b] *Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University, Houghton, MI 49931, United States*



- Carbon atom types quantified by ^{13}C and ^{1}H NMR-spectroscopy

Name	Label	Example
CH_3	CT1	
n-alkane CH_2	CT2	
iso-alkane CH	CT3	
cyclo-alkane CH_2	CT4	
cyclo-alkane to alkyl-chain CH	CT5	
cyclo-alkane to cyclo-alkane CH	CT6	
aromatic CH	CT7	
aromatic to alkyl-chain C	CT8	
aromatic to cyclo-alkane C	CT9	
aromatic to aromatic C	CT10	
aliphatic C	CT11	

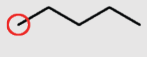
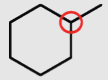
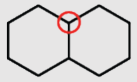
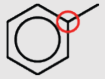
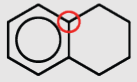


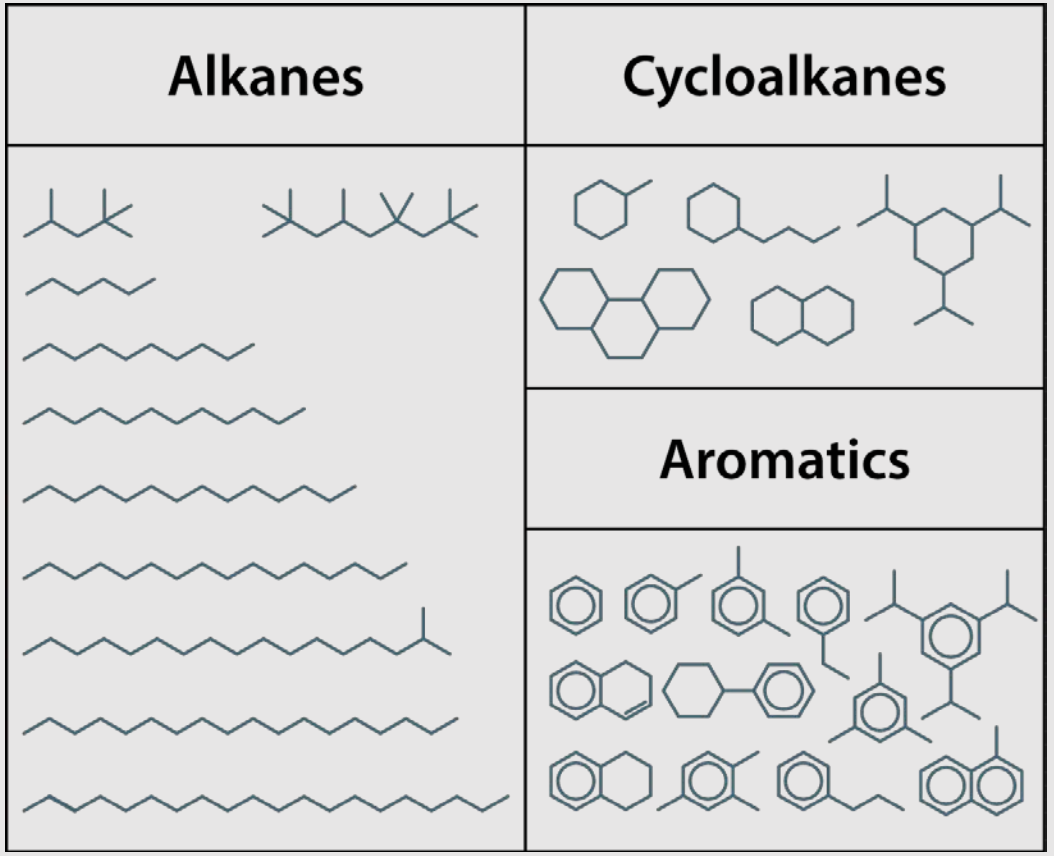
$$\mathrm{YSI} = [1] + 3[2] + 5[4] + [5]$$

$$\mathrm{YSI(predicted)} = \sum_j N_{ij}\,[\mathrm{CT}\,j]$$

$$\min \chi^2 = \sum_{i=1}^{n} [\mathrm{YSI\ (expt.)} - \mathrm{YSI\ (pred.)}]^2$$

- Carbon atom types quantified by ^{13}C and ^{1}H NMR-spectroscopy

Name	Label	Example
CH_3	CT1	
n-alkane CH_2	CT2	
iso-alkane CH	CT3	
cyclo-alkane CH_2	CT4	
cyclo-alkane to alkyl-chain CH	CT5	
cyclo-alkane to cyclo-alkane CH	CT6	
aromatic CH	CT7	
aromatic to alkyl-chain C	CT8	
aromatic to cyclo-alkane C	CT9	
aromatic to aromatic C	CT10	
aliphatic C	CT11	



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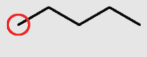
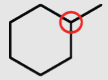
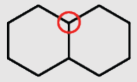
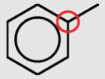
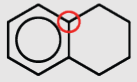
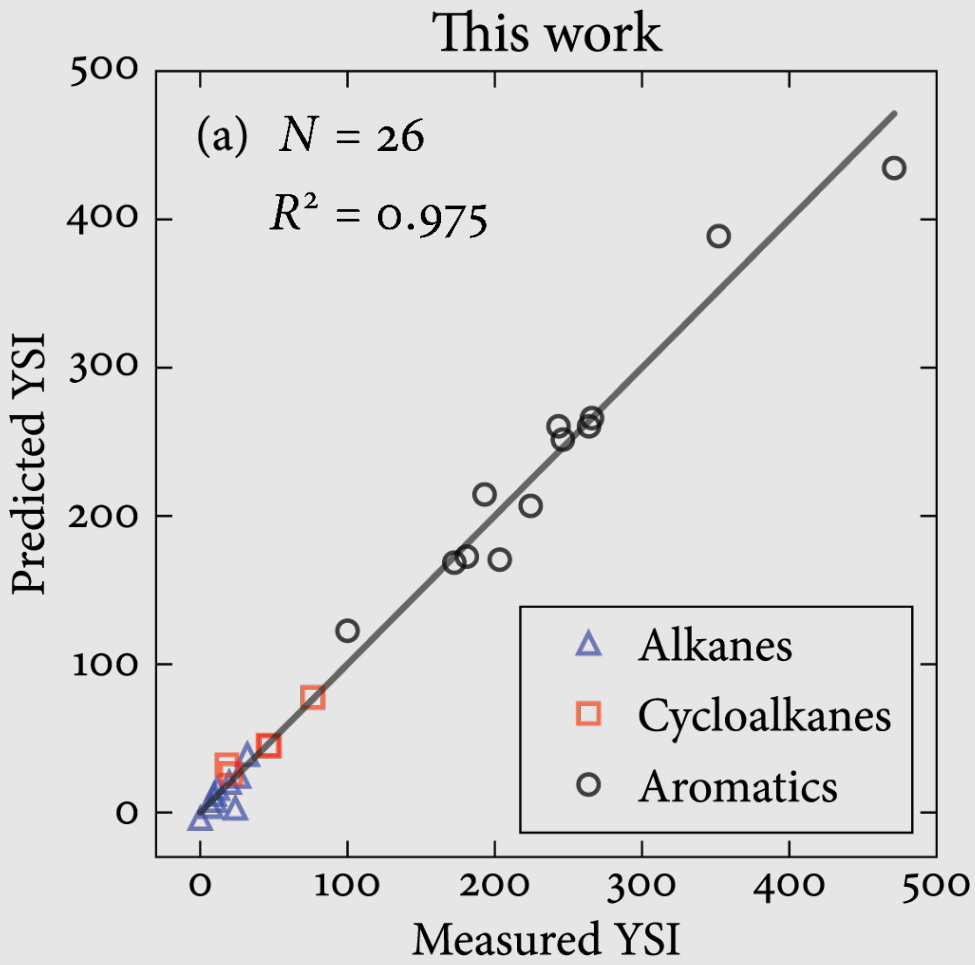
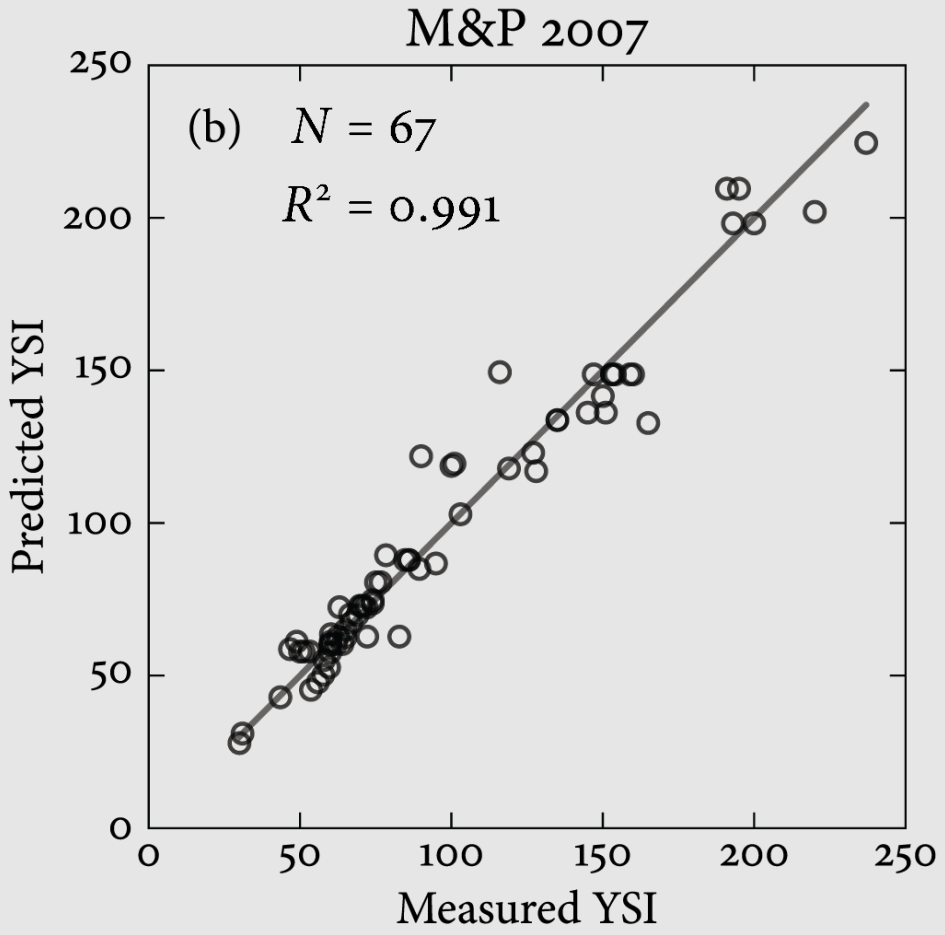
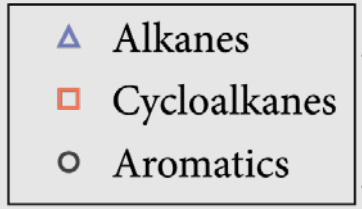
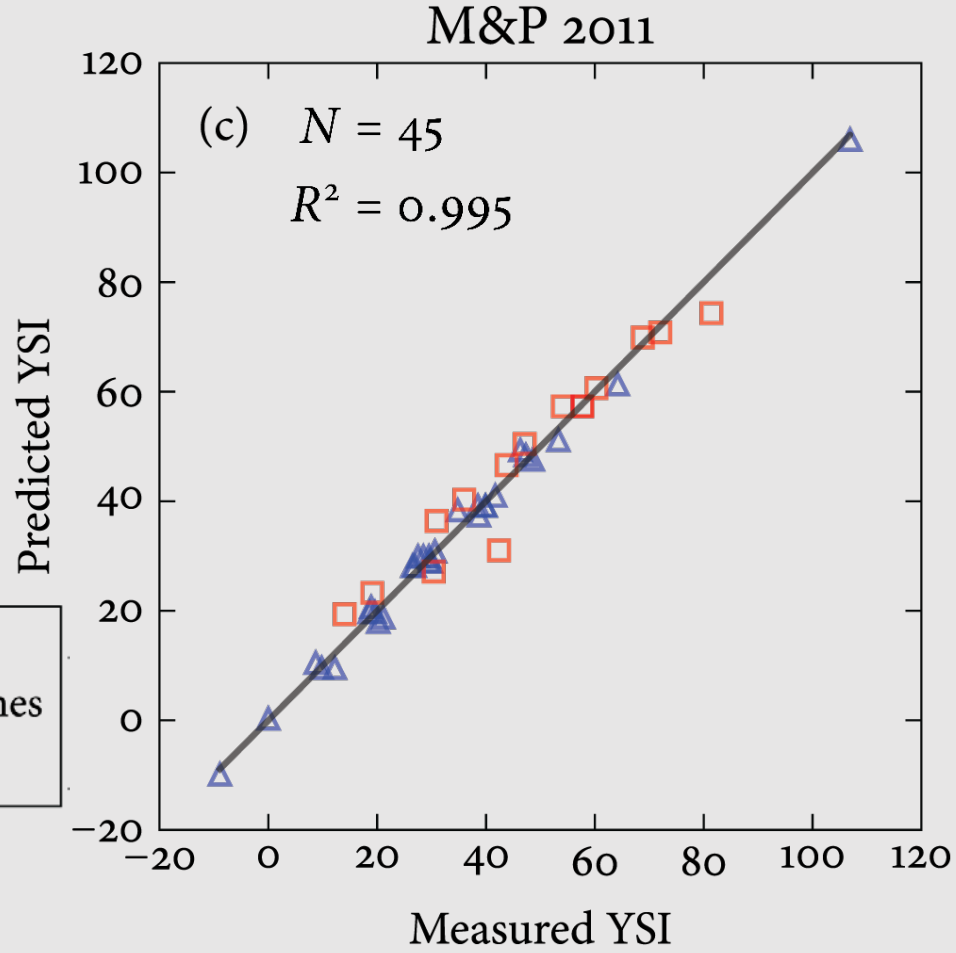
CH_3	CT1	
n-alkane CH_2	CT2	
iso-alkane CH	CT3	
cyclo-alkane CH_2	CT4	
cyclo-alkane to alkyl-chain CH	CT5	
cyclo-alkane to cyclo-alkane CH	CT6	
aromatic CH	CT7	
aromatic to alkyl-chain C	CT8	
aromatic to cyclo-alkane C	CT9	
aromatic to aromatic C	CT10	
aliphatic C	CT11	



- Carbon atom types quantified by ^{13}C and ^{1}H NMR-spectroscopy







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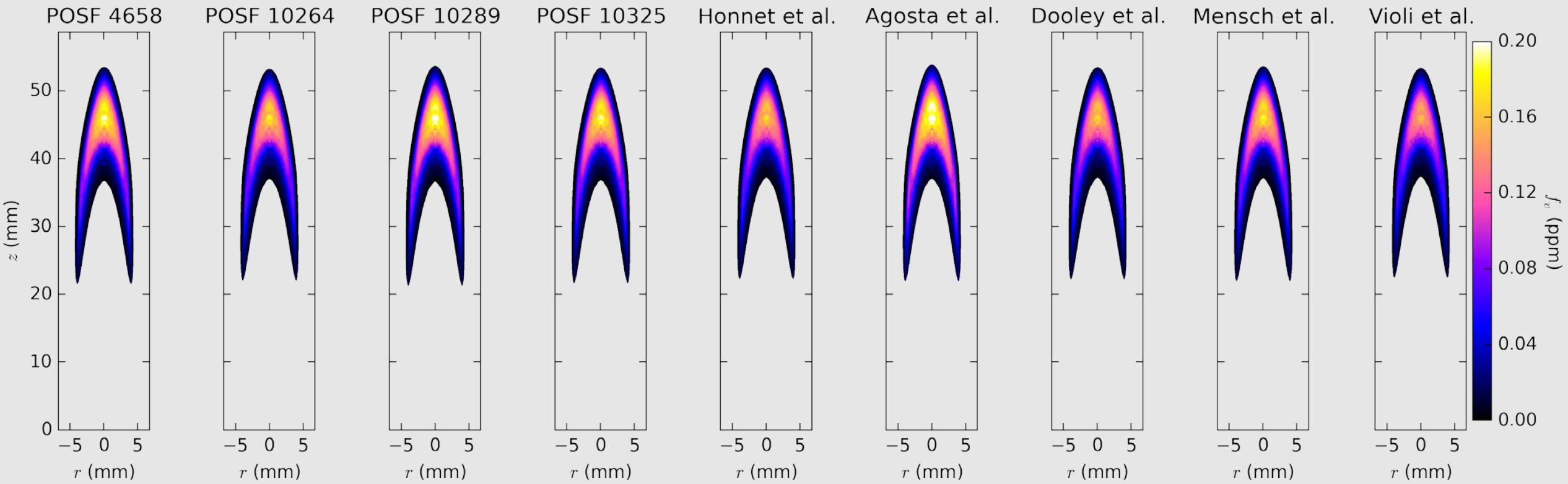
C.S. McEnally and L.D. Pfefferle, *Env. Sci. and Tech.*, 45, p 2498-503, 2011

- Predicting sooting tendencies of surrogates

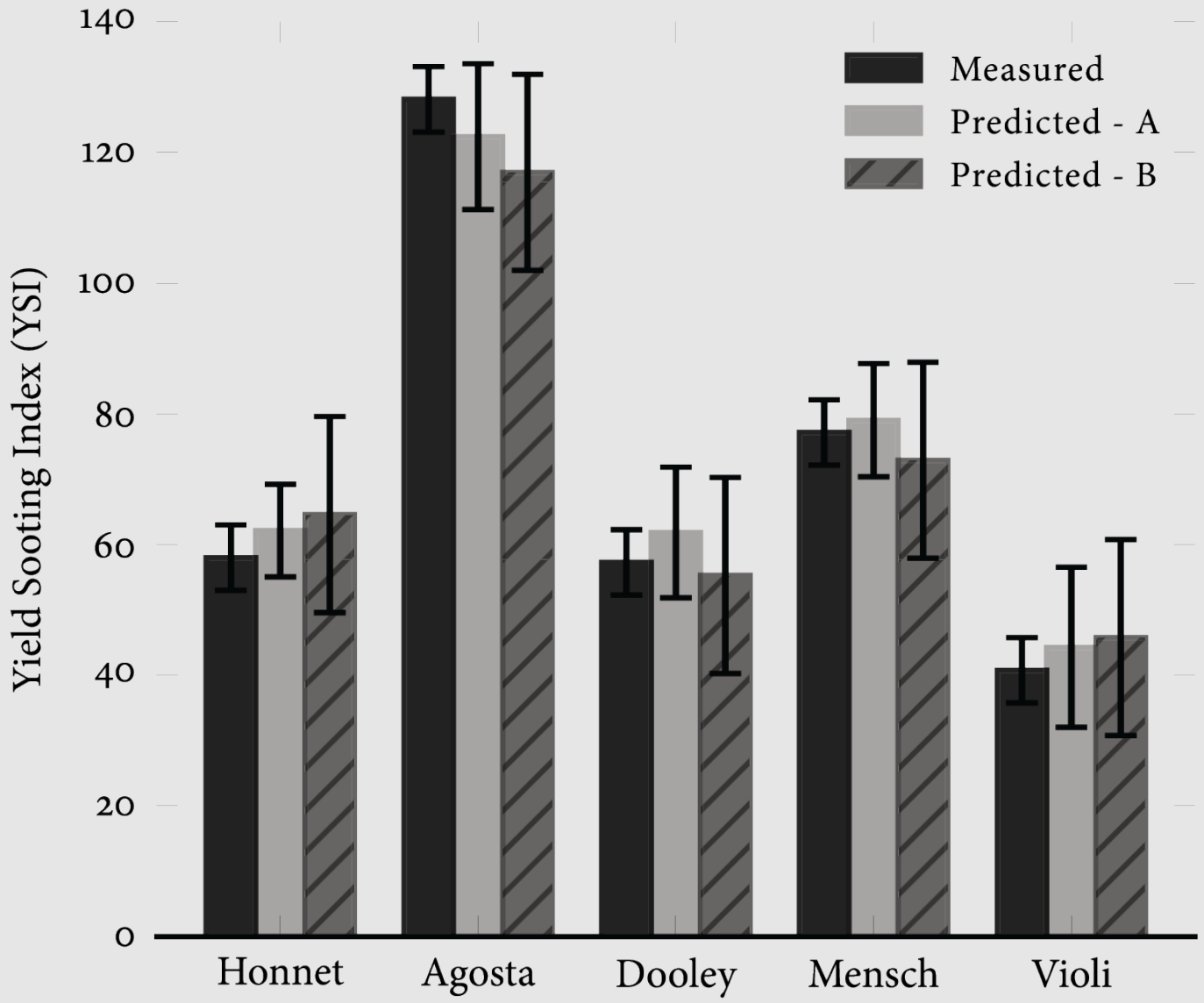
$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \mathrm{YSI_{PC}} \qquad \text{(A)}$$

$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \left(\sum_{j=1}^{11} N_j \times \mathrm{CT}_j \right)_i \qquad \text{(B)}$$

- Methane flame doped with jet fuel and surrogates



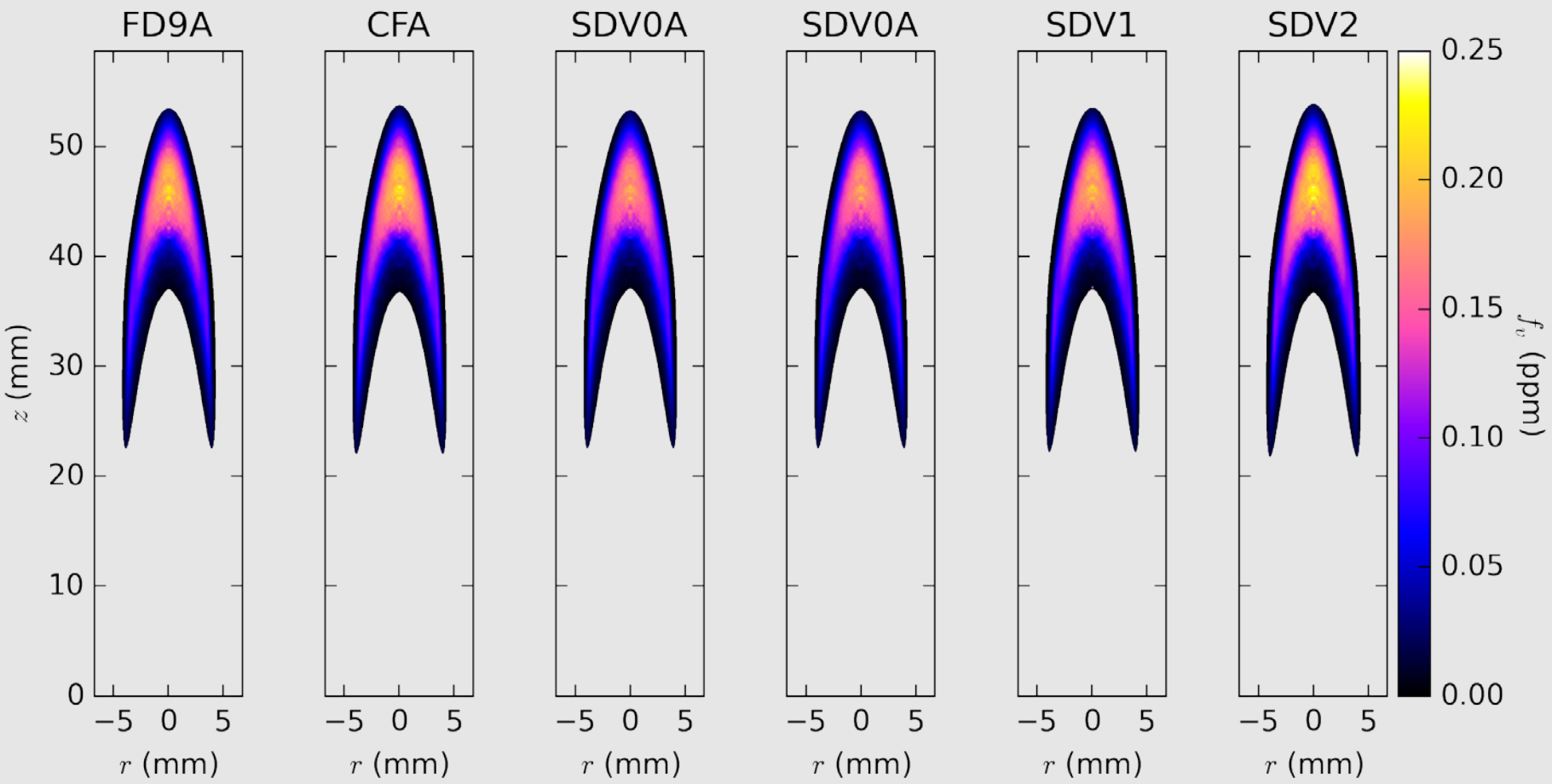
- Methane flame doped with jet fuel and surrogates



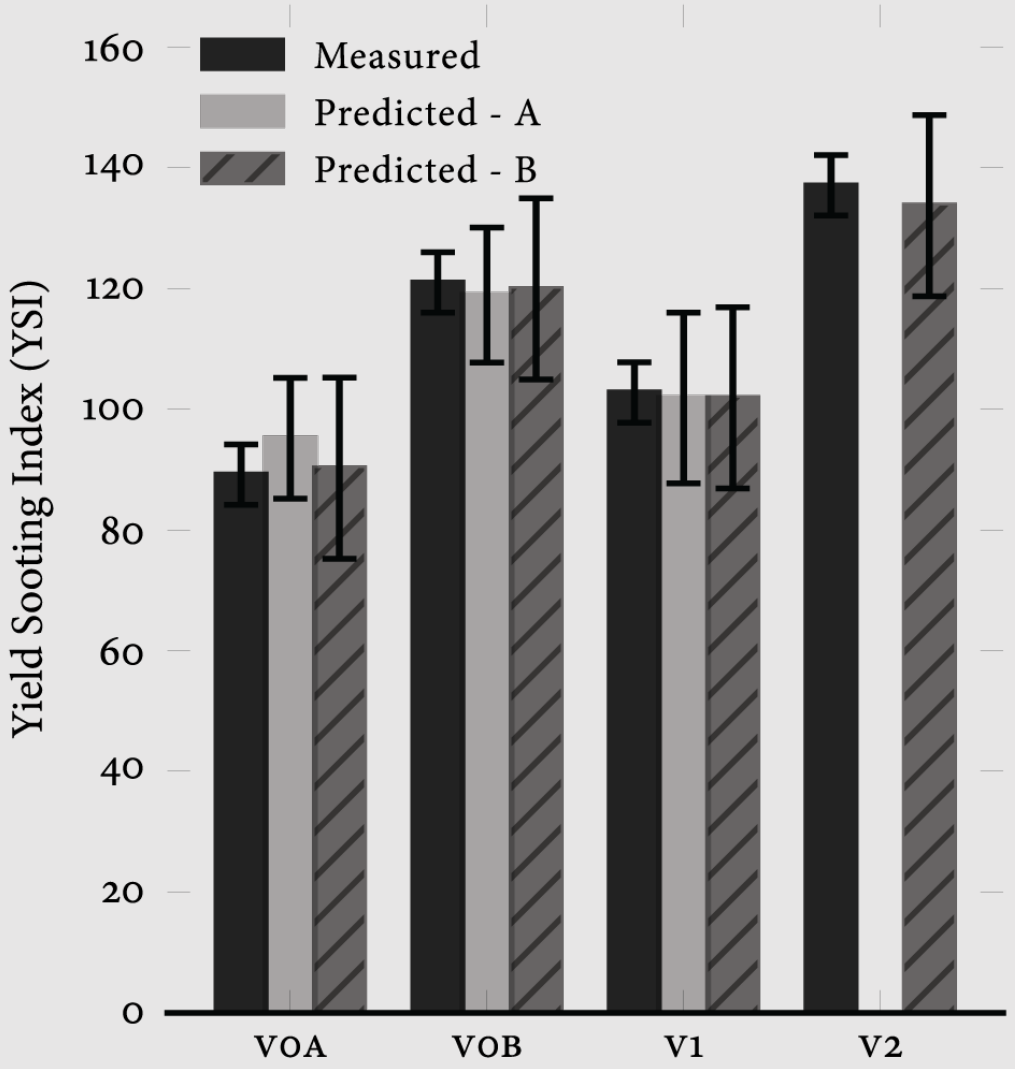
$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \mathrm{YSI_{PC}} \qquad \text{(A)}$$

$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \left(\sum_{j=1}^{11} N_j \times \mathrm{CT}_j \right)_i \qquad \text{(B)}$$

- Methane flame doped with diesel and surrogates



- Methane flame doped with diesel and surrogates



$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \mathrm{YSI_{PC}} \qquad \text{(A)}$$

$$\mathrm{YSI_{SM}} = \sum_{i=1}^{M} W_i \times \left(\sum_{j=1}^{11} N_j \times \mathrm{CT}_j \right)_i \qquad \text{(B)}$$

Summary

- Experimental technique to measure sooting tendency of low-volatility liquid fuels (~100 μL samples)
- Can measure full two-dimensional soot maps for coflow flames
- Quantified sooting tendencies of pure compounds and real fuels
- Created a 2D f_v and YSI database, can be used to develop better fuel surrogates and validate numerical soot calculations

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- Financial support from DOE/NSF Advanced Engine Combustion (award 1258654)
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- Diesel palette-compound, surrogate, and target-fuel samples from Coordinating Research Council Project AVFL-18A
- Reference jet fuel samples from Dr. Tim Edwards Air Force Research Laboratory, OH.

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