SAND2019-11861C

Understanding sources of emissions and mitigation strategies through advanced optical diagnostics and CFD simulations

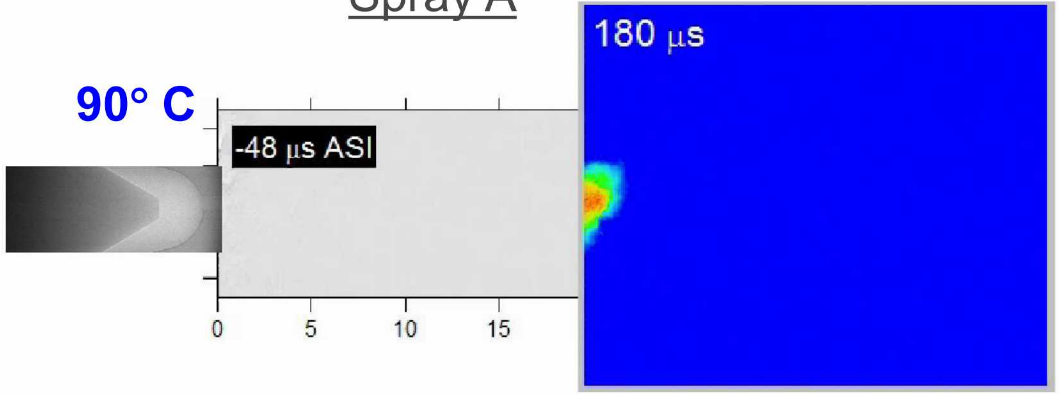
Lyle M. Pickett
Sandia National Laboratories

ENGINE COMBUSTION NETWORK

Diesel
Spray A

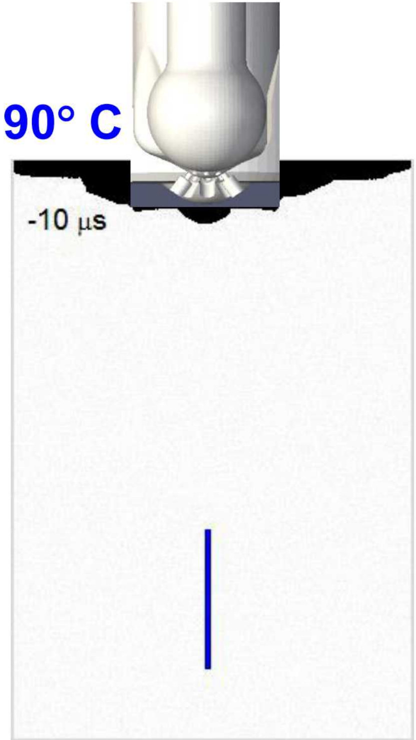
900 K
60 bar

90° C



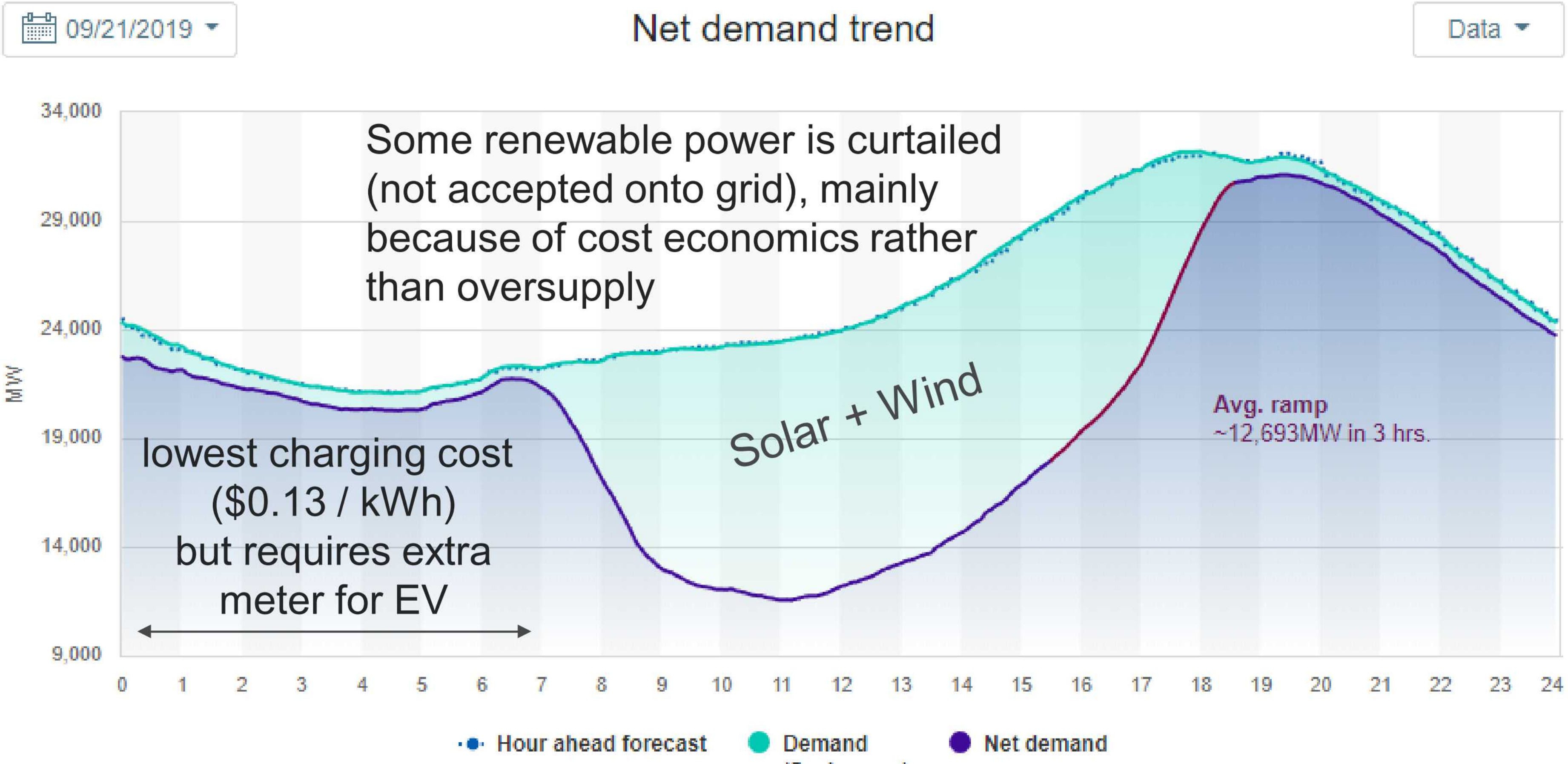
Gasoline
Spray G

90° C



573 K
6 bar

CALIFORNIA DAILY ELECTRICAL CONSUMPTION AND ELECTRICAL VEHICLE CHARGING HABITS



Comparative CO_2 emissions from ICEVs & BEVs

We compare like-functionality mid-size vehicles with a similar range

Current Day BEV:

$$CO2 = 150\ \frac{kg{-}CO2}{kWhr} * 75\ kWhr + 0.708 \frac{kg\ CO_2}{kWhr} * 26\ \frac{kWhr}{100\ mi} * 150{,}000\ \text{mi}$$

$$CO2 = 11.3 + 27.6 = \sim 39\ \text{tonnes } CO_2$$

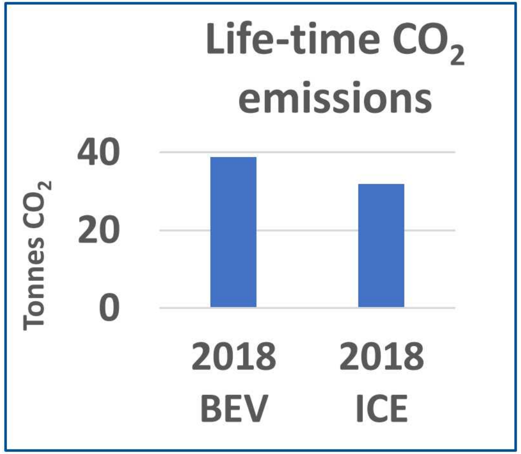
Current Day ICEV (Hybrid EV):

$$CO2 = 11.055\ \frac{kg{-}CO2}{gal} * \frac{1}{52}\frac{gal}{mi} * 150{,}000\ \text{mi}$$

$$CO2 = \sim 32\ \text{tonnes } CO_2$$

Assumptions:

- 2018 US average marginal emissions rate = 0.708 kg CO_2/kWhr per EPA AVERT model
- Emissions associated with battery manufacture = 150 kg-CO2e/kWhr; 75 kWhr battery; no replacement battery
- Energy requirements for BEV = 26 [KW-hr/100 mi] (Tesla Model 3 2018)
- Carbon intensity of gasoline = 11.055 kg-CO2/gal (GREET 2018)
- 2018 Camry Hybrid 5-cycle fuel economy = 52 mpg
- 150,000 mi lifetime ~25-yr NHTSA survivability weighted estimate



How might this change looking forward to 2050?

Future BEV:

$$CO2 = 100\ \frac{kg{-}CO2}{kWhr} * 75\ kWhr + 0.460\ \frac{kg\ CO_2}{kWhr} * 22\ \frac{kWhr}{100\ mi} * 150{,}000\ \text{mi}$$

$CO2 = 7.5 + 15.2 =$ 22.7 tonnes CO_2

Future ICEV (HEV):

$$CO2 = 11.055\ \frac{kg{-}CO2}{gal} * \frac{1}{75}\frac{gal}{mi} * 150{,}000\ \text{mi}$$

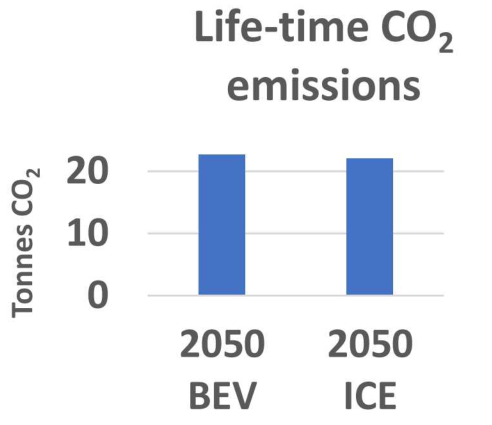
$CO2 =$ 22.1 tonnes CO2

Assumptions:

- Future US average marginal emissions rate = 0.460 kg CO_{2e}/kWhr
- Emissions associated with battery manufacture = 100 kg-$CO2_e$/kWhr; 75 kWhr battery; no replacement battery
- Energy requirements for BEV = 22 [KW-hr/100 mi]
- Carbon intensity of gasoline = 11.055 kg-CO2/gal (GREET 2018)
- 150,000 mi lifetime close to 25-yr NHTSA survivability weighted estimate

Conclusion

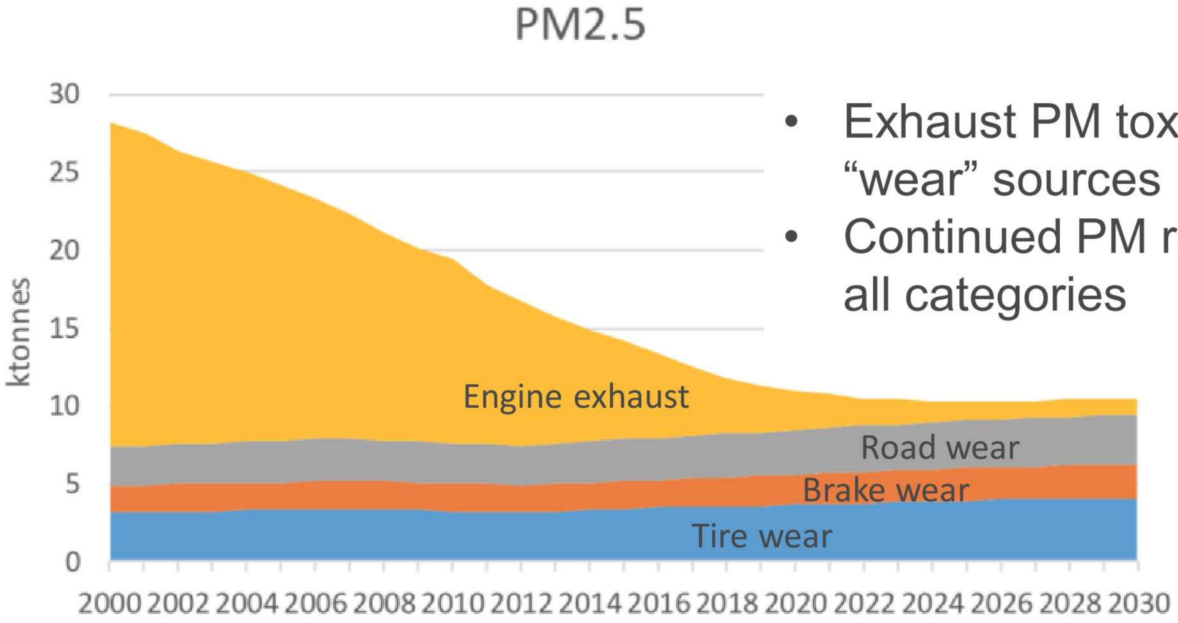
- In the short-term in the US, BEVs offer no CO_2 emission benefits over HEVs (or even 41 mpg conventional ICEs)
- Looking to the future, we can expect approximate parity between the two technologies



ENGINE EMISSION CONTROLS DRAMATICALLY DECREASE THE IMPACT OF EXHAUST PARTICULATE MATTER ON AIR QUALITY

Air Quality Expert Group report for the United Kingdom, 2019

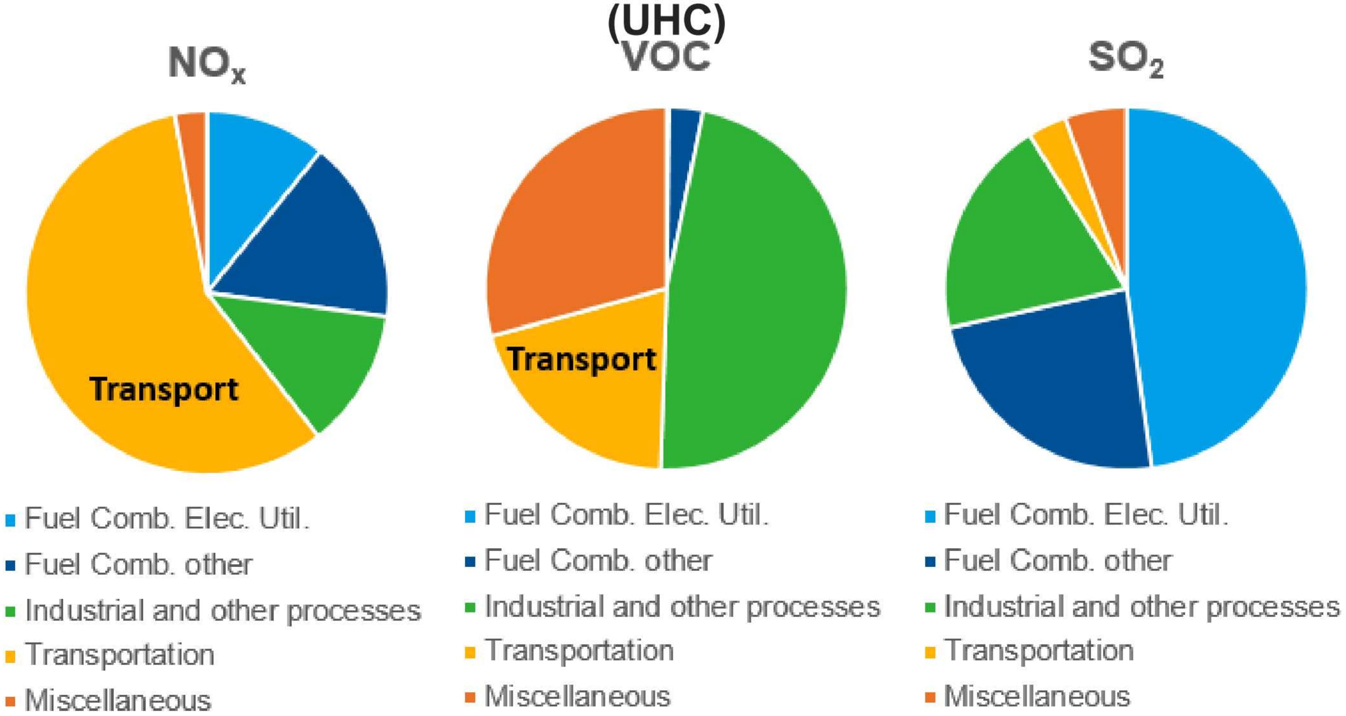
https://uk-air.defra.gov.uk/assets/documents/reports/cat09/1907101151_20190709_Non_Exhaust_Emissions_typeset_Final.pdf



- Exhaust PM toxicity may be greater than "wear" sources
- Continued PM reduction is desirable in all categories

NITROGEN OXIDE AND UNBURNED HYDROCARBON CONTRIBUTIONS FROM TRANSPORTATION ARE SIGNIFICANT

2018 emissions from EPA National Emission Inventory



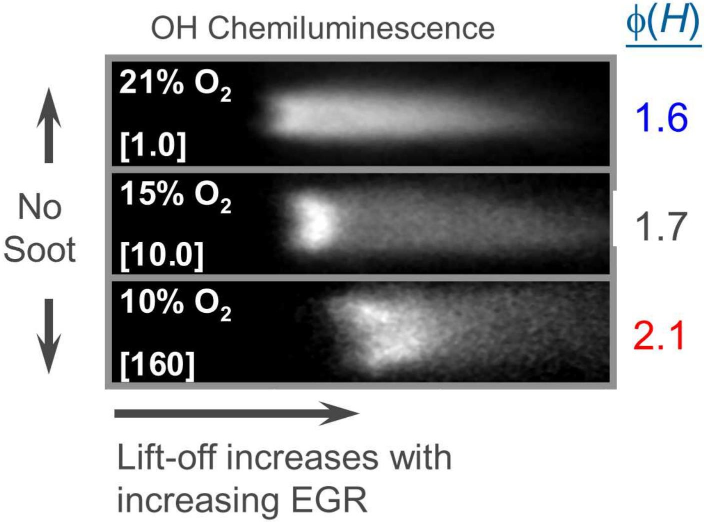
CRITICAL NEED TO IMPROVE EFFICIENCY WHILE BRINGING ICE EMISSIONS (SOOT, NOX, UHC) TO "ZERO-IMPACT"

- Together we can facilitate the development of clean, efficient, low-cost engines
  – Predictive spray, engine flows, and combustion is key
  – Applies to all classes of engines
- Even with massive battery electric emergence, there will be 1 billion new ICEs made between now and 2040—let's make these 1 billion ICEs better[1]

[1] SAE Automotive International quotation of TULA President Scott Bailey

ENGINE COMBUSTION NETWORK

SOOT-FREE, LOW TEMPERATURE COMBUSTION USING EGR AND FAST MIXING WITH MIXING-CONTROLLED HEAT RELEASE (IN SPRAY CHAMBER)



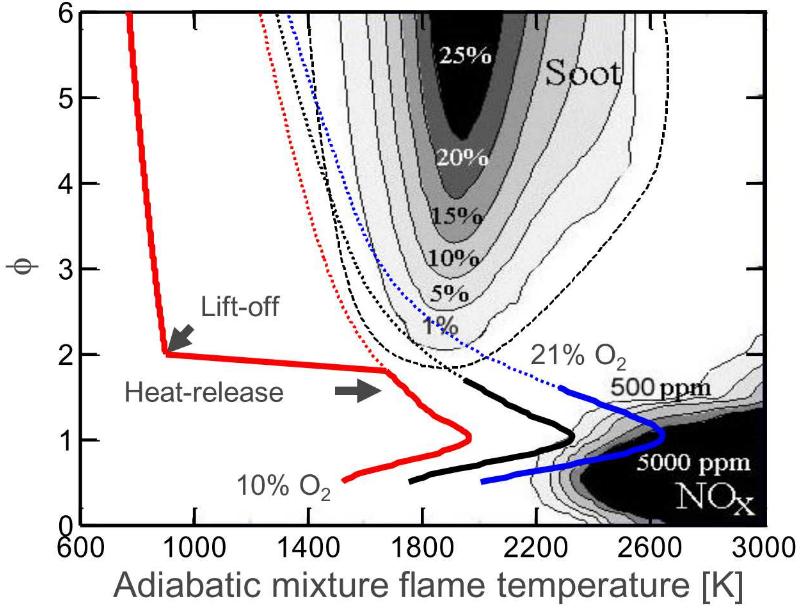
Pickett, SAE 2004-01-1399

<u>Single, isolated fuel spray conditions:</u>

T_a: 1000 K

d: 50 μm

Fuel: #2 diesel



- How to realize and optimize such clean combustion in a realistic engine?

COLLABORATIVE RESEARCH THROUGH THE ENGINE COMBUSTION NETWORK ACCELERATES CFD MODEL DEVELOPMENT

ENGINE COMBUSTION NETWORK

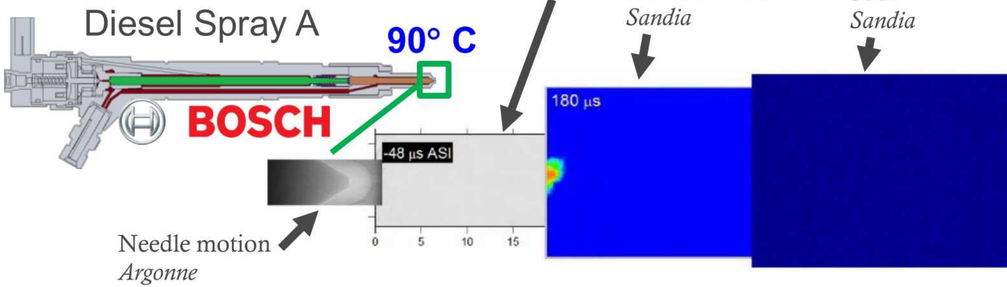
Approach

- Develop diesel and gasoline target conditions with emphasis on CFD modeling shortcomings
- Comprehensive experimental and modeling contributions
- Diesel Spray A, B, C, D
- Gasoline Spray G
- Results submitted to online archive (ecn.sandia.gov) with fields (like geometry and uncertainty) specifically tailored for CFD simulations

Impact

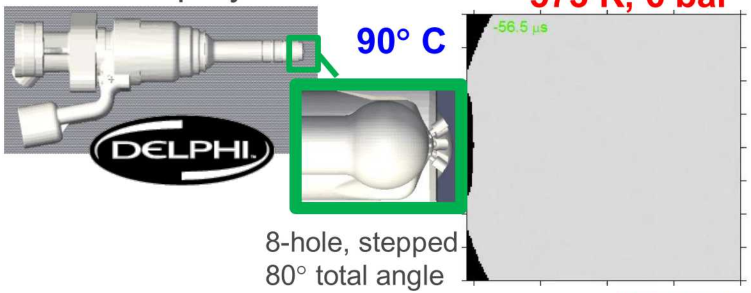
- Established in 2009, there are already 1400 citations of the ECN data archive
- Most automotive industry (light- and heavy-duty) use ECN archive to test their own CFD methods

ECN formed in 2009



>70 measurements/diagnostics contributed from >15 institutions

900 K
60 bar



ENGINE COMBUSTION NETWORK

ECN CONTRIBUTORS FOR THIS TALK

- Julien Manin, Scott Skeen, Jonathan Frank, Mark Musculus, Emre Cenker, Joonsik Hwang, Marco Arienti, Rainer Dahms, *Sandia National Laboratories*
- Gilles Bruneaux, Louis-Marie Malbec, Michele Bardi, *IFP Energies nouvelle*
- Raul Payri, José M. García-Oliver, Pedro Martí-Aldaraví, Jesús Benajes, José M. Desantes, J. Javier López, Darío López-Pintor, *CMT Motores Térmicos*
- Evatt Hawkes, *UNSW Australia*
- Noud Maes, Maarten Meijer, Nico Dam, Bart Somers, *Tech. Univ. of Eindhoven*
- Chris Powell, Alan Kastengren, Daniel Duke, Katie Matusik, Sibendu Som, Yuanjing Pei, Kaushik Saha, *Argonne National Laboratory*
- Cyril Crua, *Univ. Brighton*
- Fredrik Westlye, *Tech Univ. Denmark*
- Michele Battistoni, *Univ. Perugia*
- Panos Sphicas, *Imperial College London*
- Tim Bazyn, Glen Martin, Russ Fitzgerald, *Caterpillar Inc.*
- Scott Parrish, Ron Grover, *GM R&D*
- Tommaso Lucchini, David Sinoir, Davide Paredi, Gianluca d’Errico, Politecnico di Milano (PoliMi)
- Hong G. Im, F. E. Hernandez Perez, *KAUST*
- Chris Rutland, Hongjiang Li, *Univ. of Wisconsin-Madison*
- Jihad A. Badra, Jaeheon Sim, *AramCo*

ENGINE COMBUSTION NETWORK

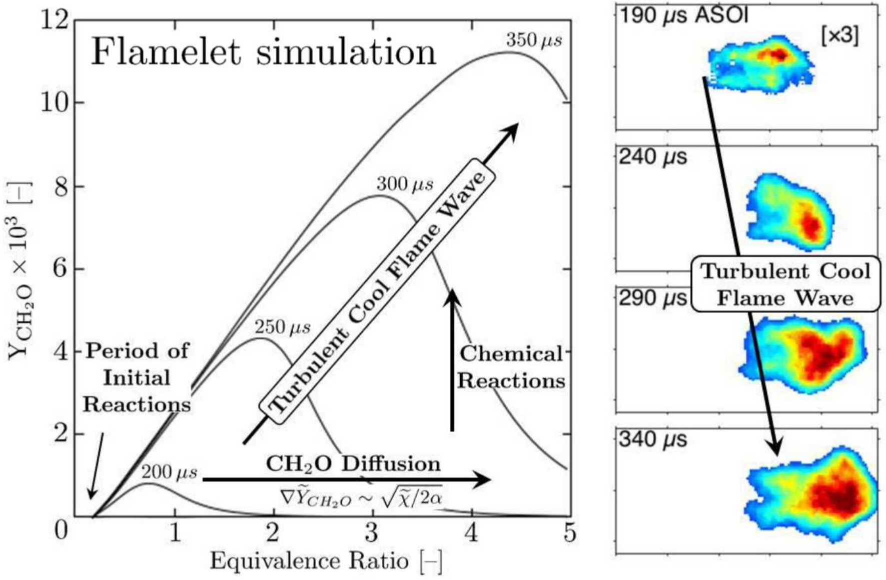
ACKNOWLEDGEMENTS

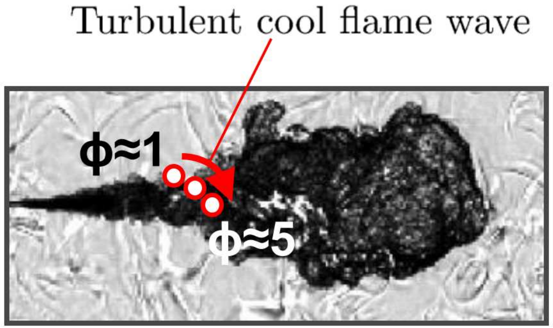
- Gurpreet Singh, Mike Weismiller, Kevin Stork, *Funding for Sandia contribution provided by US DOE Office of Vehicle Technologies*
- *French Ministry of Ecology, Energy, Sustainable Development and Sea*
- David Cook, Godehard Nentwig, Joel Oudart, Ed Knudsen, *Robert Bosch LLC*, *donation of injectors*.
- Dan Varble and Lee Markle, *Delphi, donation of injectors.*

ENGINE COMBUSTION NETWORK

IGNITION MECHANISM ANALYSIS FOR SPRAY A

→ Turbulence generates *steep* gradients and, hence, strong diffusion fluxes





see Dahms, Paczko, Skeen, Pickett. ProCI 36(2), 2017

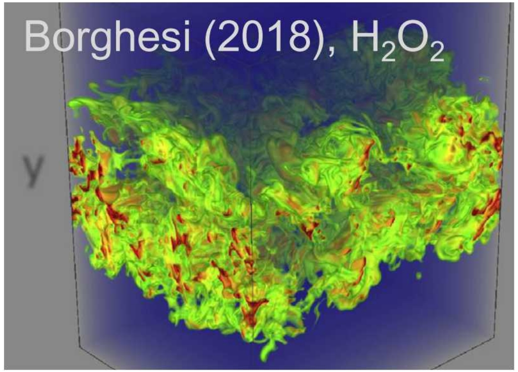
<u>Effect</u>:

a) Species & temperature diffusion into neighbored mixture triggers 1st-stage ignition

b) Continuous reactions & diffusion leads to cool flame "wave" propagation

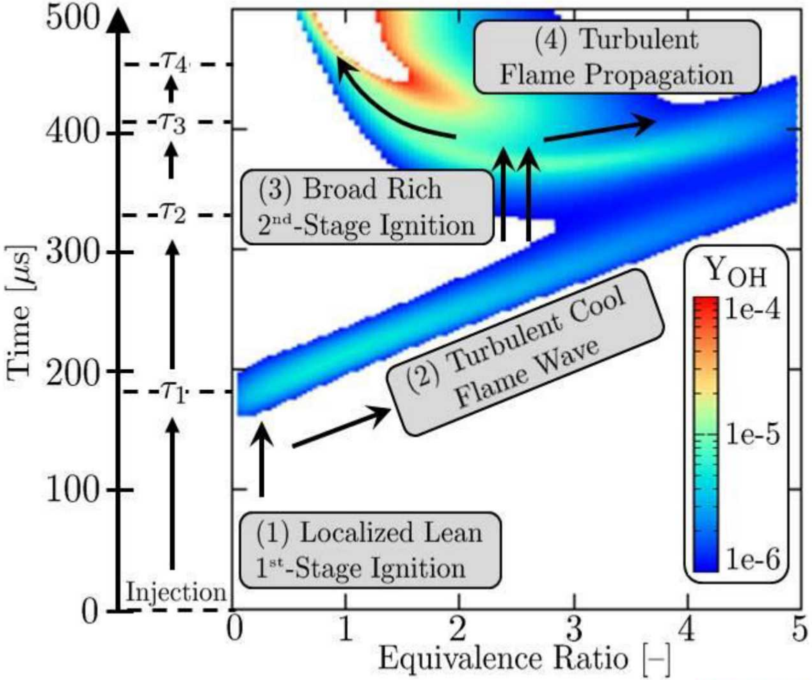
TRANSPORT OF COOL-FLAME SPECIES AND T CREATES BROAD MIXTURES FOR SECOND-STAGE HIGH-T IGNITION

- CFD researchers showing cool flame accelerating rich ignition:
  - Gong (2014) & Pei (2015) (both using 3D LES, homogenous reactor combustion)
  - Krisman & Hawkes (2017), 2D DNS
  - Borghesi (2018), temporally evolving 3D DNS (65 million CPU-hrs)



n-dodecane
25 bar
T_{amb} = 960 K
35 species reduced mechanism

Dahms (2017) conceptual model based on full-chemistry flamelet analysis

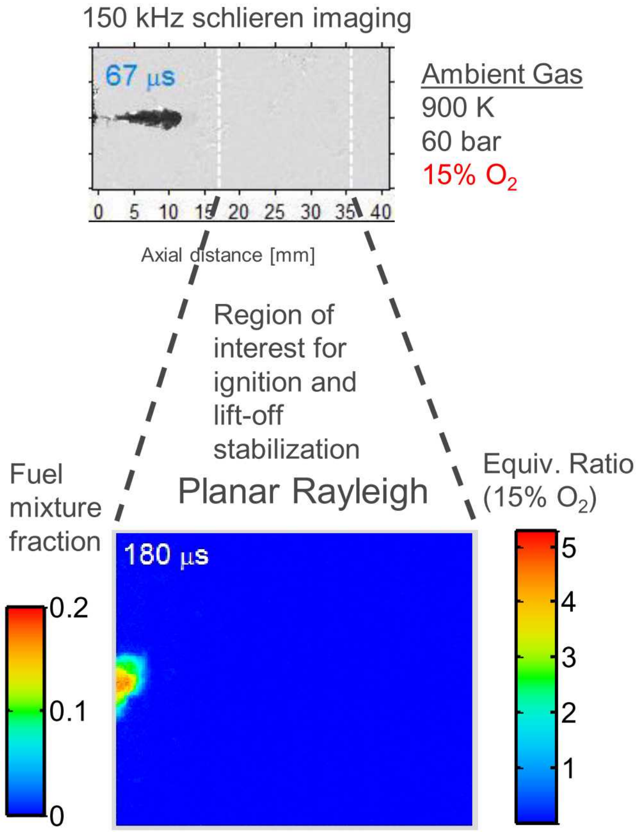


TRANSIENT SPRAY MIXTURE FRACTION MEASURED (NON-REACTING) IN VAPORIZED REGION

- Apply custom pulse-burst laser
- Jet mixing characterized by large structures shed to the side and re-entrained
  - Larger residence time in hot mixtures
- Obvious target for high-fidelity LES studies
  - verify accurate mixing field as a preliminary step towards predicting ignition/combustion
  - quantify variance, intermittency, scalar gradients

Parameter	Quantity
Frequency	100 kHz
Burst duration	5 ms
Pulse width	4 – 8 ns
Wavelength	532 nm
Pulse energy	15 mJ
Polarization	Horizontal

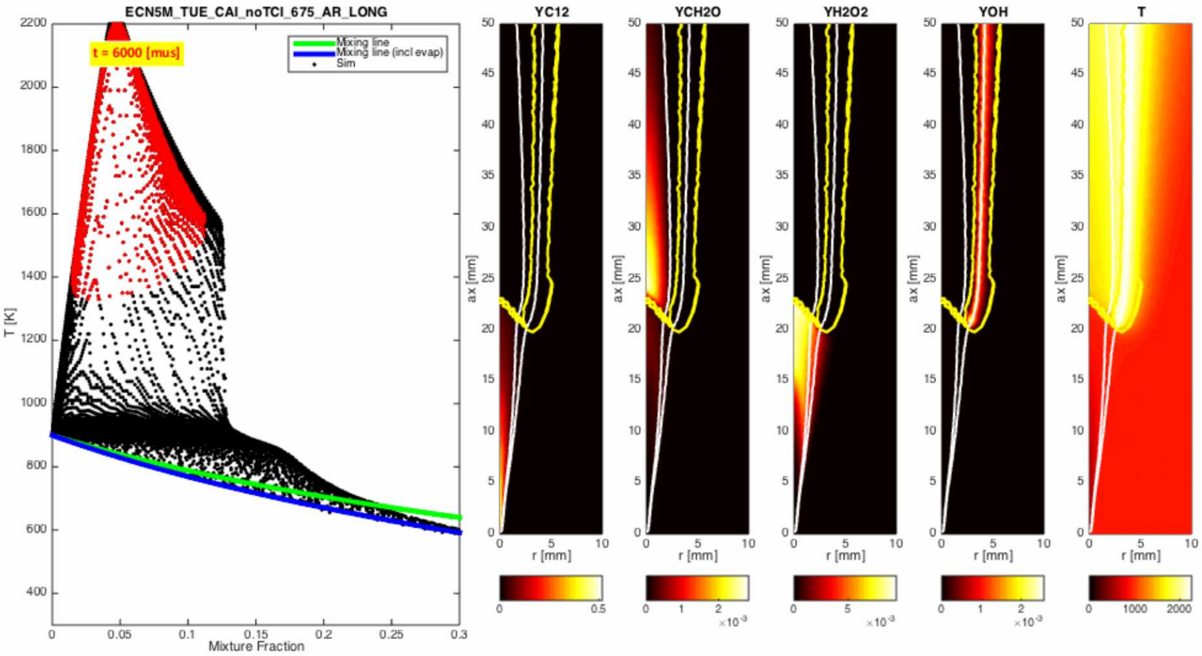
Julien Manin et al., Sandia, 2017



Ambient Gas
900 K
60 bar
0% O_2

COMPARISON OF MEASURED OH AND FORMALDEHYDE CH2O VERSUS SIMULATION

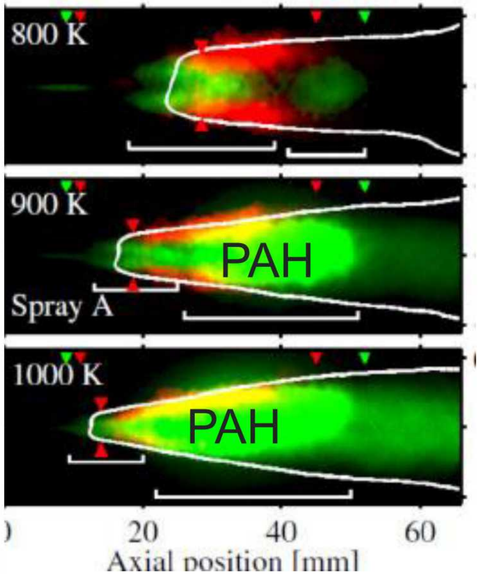
900 K: TUE, Flamelet Generated Manifold, OpenFOAM



TU/e experiment

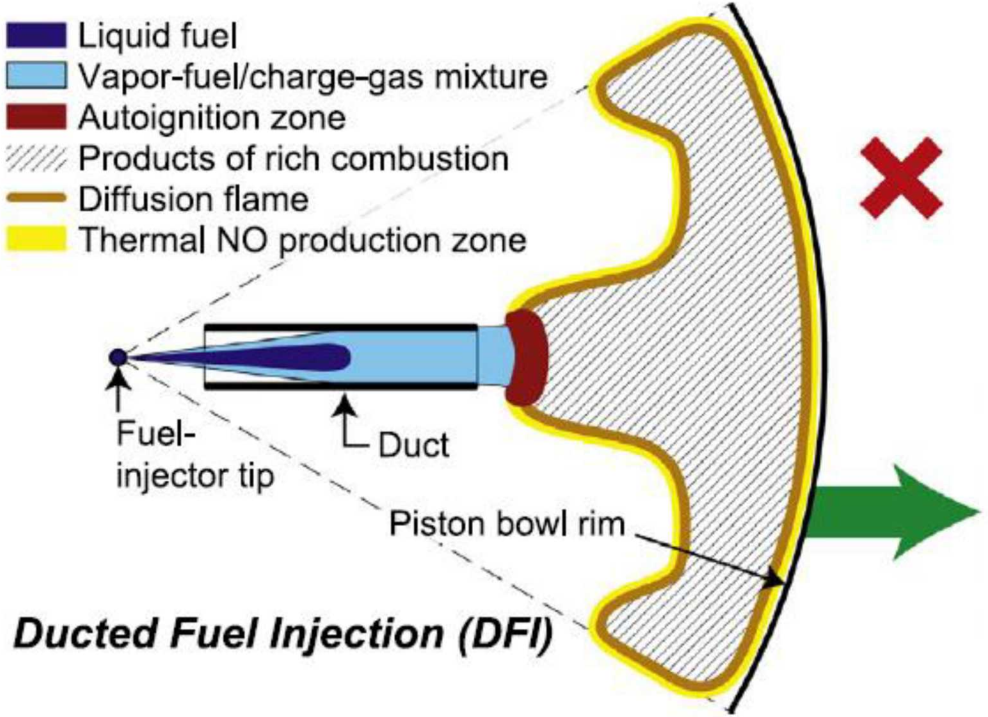
Green: planar CH2O

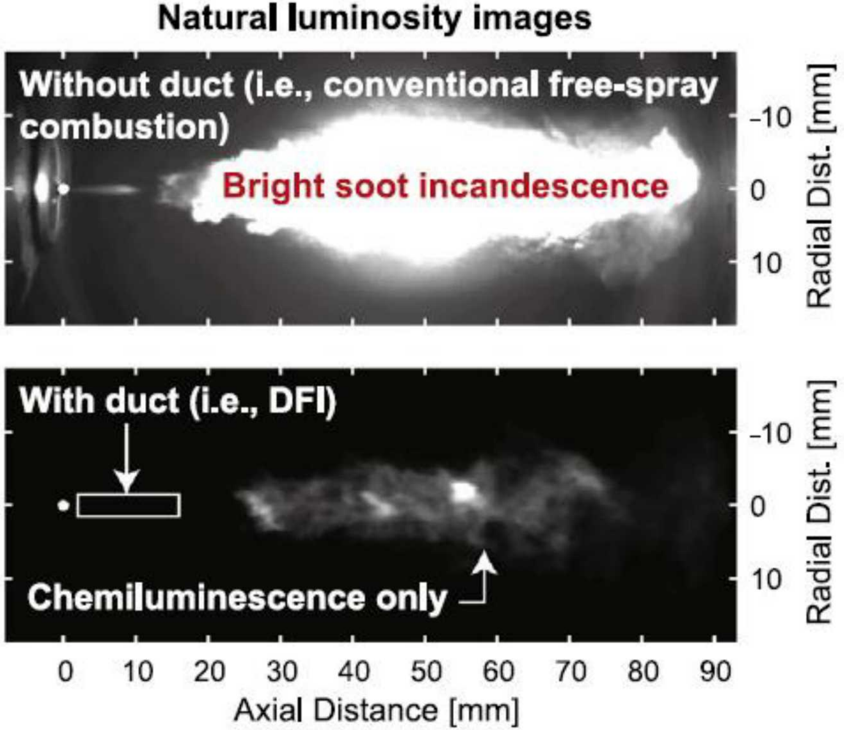
Red: planar OH



ENGINE COMBUSTION NETWORK

ACHIEVING SOOT-FREE, LOW-T COMBUSTION USING DUCTED FUEL INJECTION





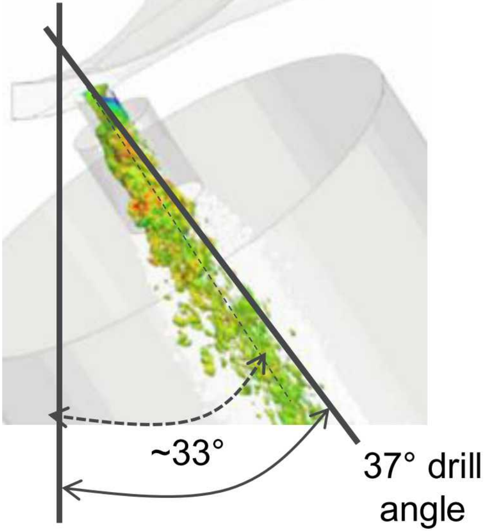
CJ Mueller et al. 2017, Sandia

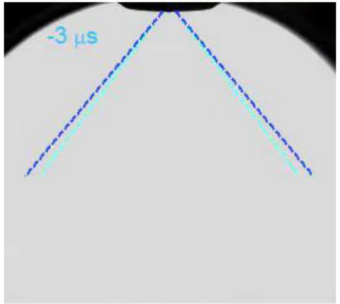
Spray A with a duct – soot free!

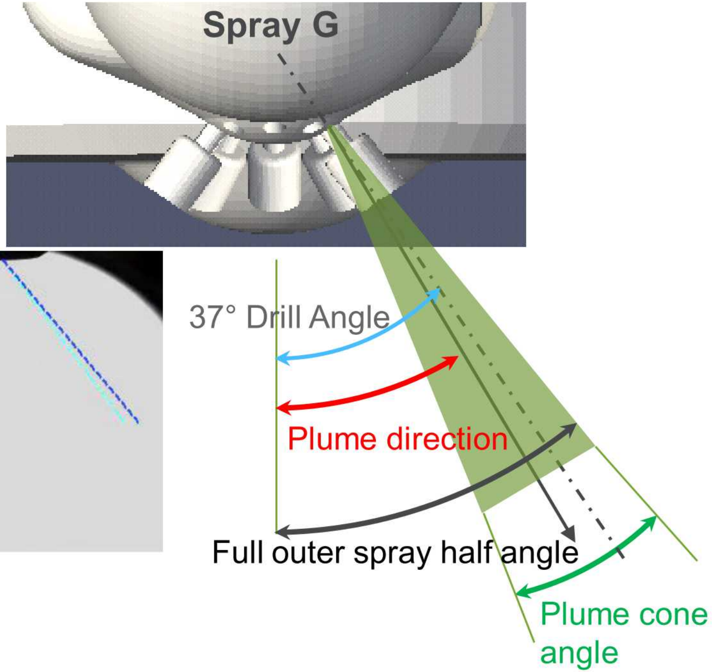
CRITICAL ISSUE FOR GDI: PREVENTING LIQUID IMPINGEMENT AND MIXING IMPERFECTIONS

VOF simulation of internal flow

ECN4: courtesy Bizhan Befrui, Delphi

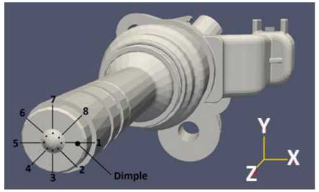




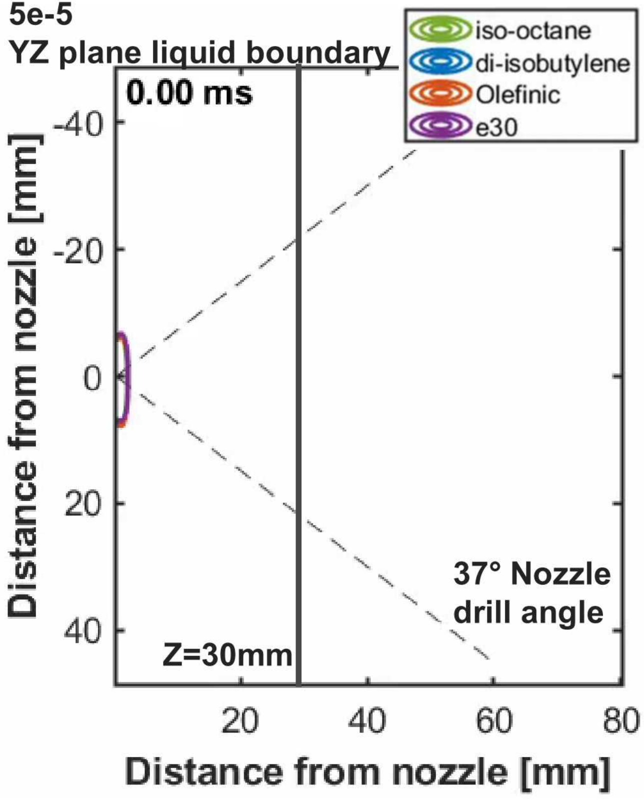


- Changes expected during injection:
  - "Plume direction" angle relative to injector
  - Individual plume "cone angle"
- Predicting plume direction, growth, and interaction is complex

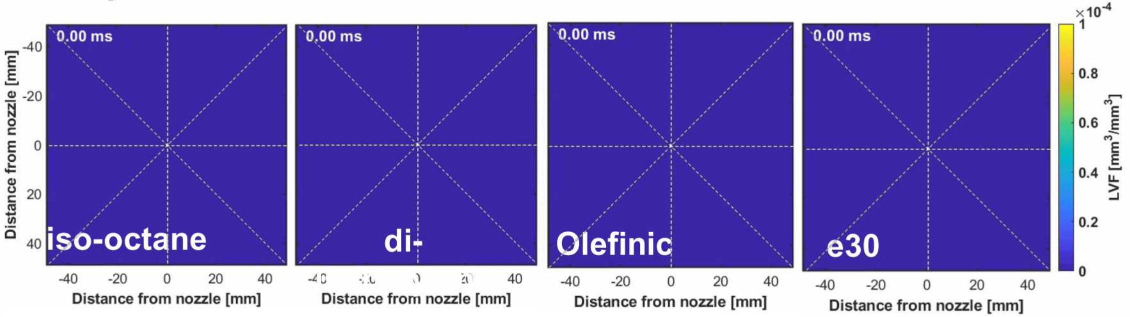
EFFECTS OF FUEL ON PLUME MOVEMENT FOR SPRAY G (0.5 BAR AMBIENT—FLASH BOILING)



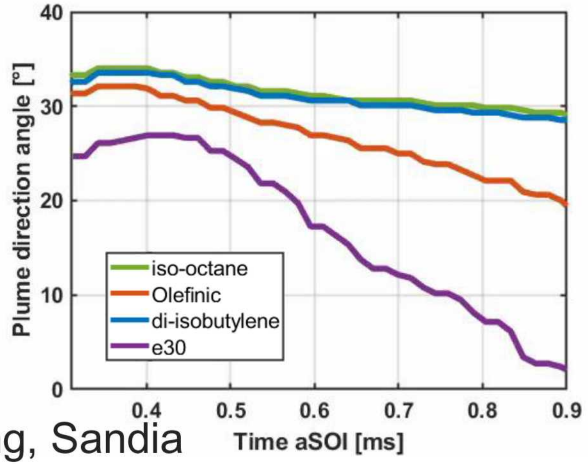
Liquid volume fraction threshold 5e-5
YZ plane liquid boundary



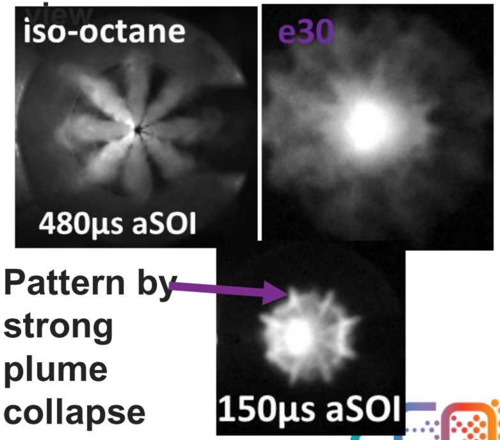
Liquid volume fraction at Z=30mm



Plume direction angle at Z=30mm

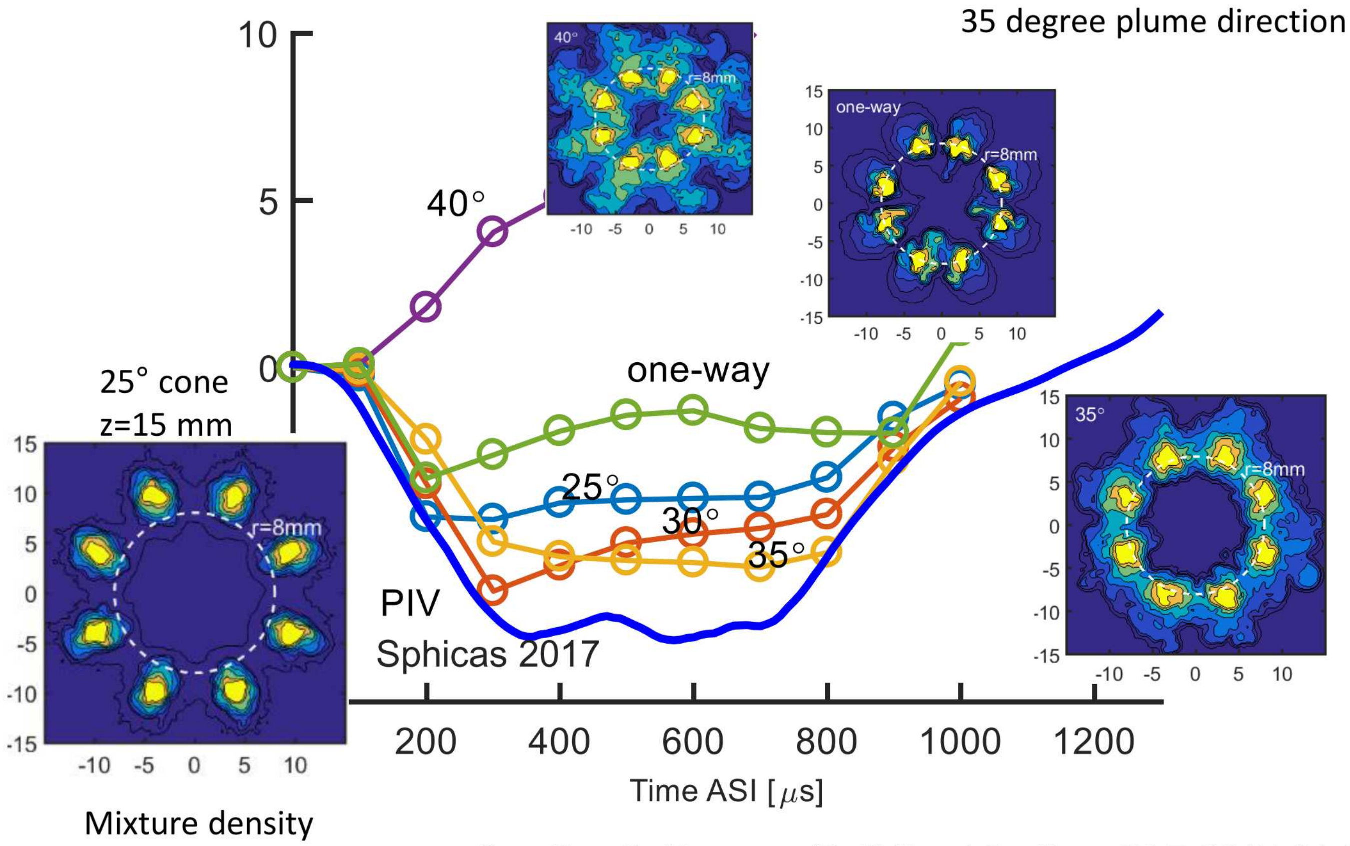


Mie-scattering image at front view



Planar data after CT of spray; Hwang, Sandia

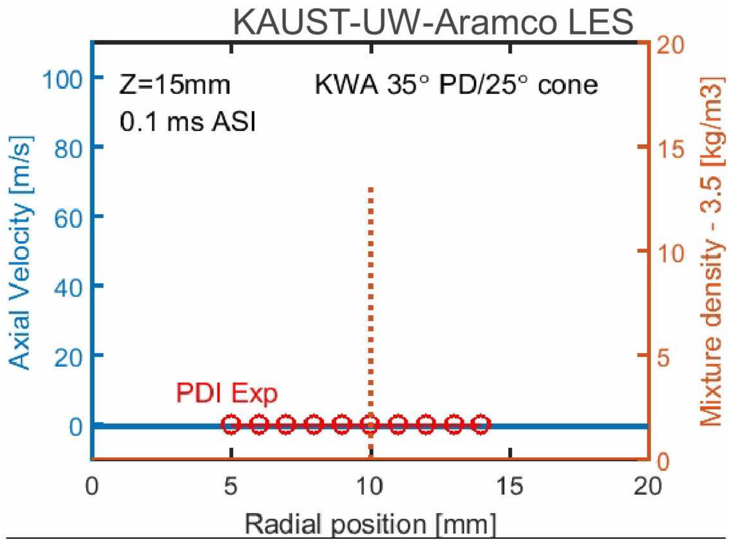
ARGONNE LES: EXPERIENCES A TOGGLING/COLLAPSE WITH INCREASED PLUME CONE ANGLE



See Sandia/Argonne/PoliMi publication: SAE 2017-01-0837

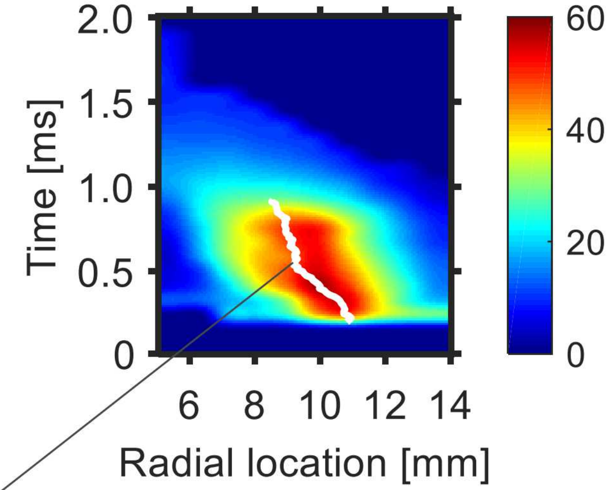
AFTER CHOOSING PLUME CONE ANGLE CASE WITH THE BEST MATCH TO EXPERIMENT GAS VELOCITY:

- Nice agreement with measured liquid velocity
- Plume center moves towards injector axis during injection
- Plume center measured with DBI extinction imaging also consistent



Average of all 8 plumes, and average of 5 LES realizations

Measured liquid velocity magnitude by phase-Doppler interferometry Scott Parrish (GM)



Plume center from Sandia extinction imaging

ENGINE COMBUSTION NETWORK

COUPLING EXPERIMENTAL AND MODELING EFFORTS HOLDS POTENTIAL TO OVERCOME EMISSIONS CHALLENGES FOR ICEs

- Diesel:
  - ECN experiments and simulations (even DNS) suggest important cool-flame transport as key to turbulence chemistry interaction
  - Soot-free combustion with control is possible
- Gasoline:
  - Interaction between plumes must be predicted to minimize wall impingement

감사합니다

- Questions?