SAND2016-10819C

The role of turbulence and cool-flame kinetics in high-pressure spray ignition

Rainer N. Dahms[1], Günter A. Paczko[2], Scott A. Skeen[1], and Lyle M. Pickett[1]
[1]*Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA*
[2]*Institute for Combustion Technology, RWTH Aachen University, Germany*

U.S. DEPARTMENT OF ENERGY | Office of Science | Energy Efficiency & Renewable Energy
VEHICLE TECHNOLOGIES OFFICE

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences and Office of Vehicle Technologies

Synopsis

- This work seeks a first-principles understanding of two-stage ignition mechanism in high-pressure spray combustion

A. Experiments:
Quantitative time scales & spatial progression of ignition from simultaneous formaldehyde PLIF & schlieren images

B. Theoretical-numerical modeling:
Establishing the validity of the flamelet eqns & full LLNL reference kinetics for high-pressure low-temperature combustion

- Ignition mechanism in turbulent high-pressure flames
  - "Turbulent cool-flame wave" & impact on turbulent ignition
  - Fundamental time scales in high-pressure spray ignition
  - Sensitivity to fluctuations in scalar dissipation rates

(Some) Review on relevant LTC studies

Prior fundamental studies have investigated the impact of cool-flame chemistry

- Counterflow experiments/computations/asymptotics at elevated pressures
  (Seshadri *et al*., Combust. Theory Modelling, 2016)
- Micro-gravity droplet combustion experiments at intl. space station
  (Nayagam *et al*., Combust Flame, 2012; Farouk & Dryer, Combust. Flame, 2014)
- DNS of droplet combustion without flow or turbulence
  (Borghesi *et al*., Combust. Flame, 2013)
- DNS has shown ignition in preferably rich mixtures
  (Mukhopadhyay and Abraham, Combust. Flame, 2012; Viggiano, Combust. Flame, 2010)
- Most recent DNS & LES results indicate importance of cool-flame in ignition
  (Krisman *et al*. Combust. Flame, 2016; Pei *et al*., Combust. Flame, 2016)

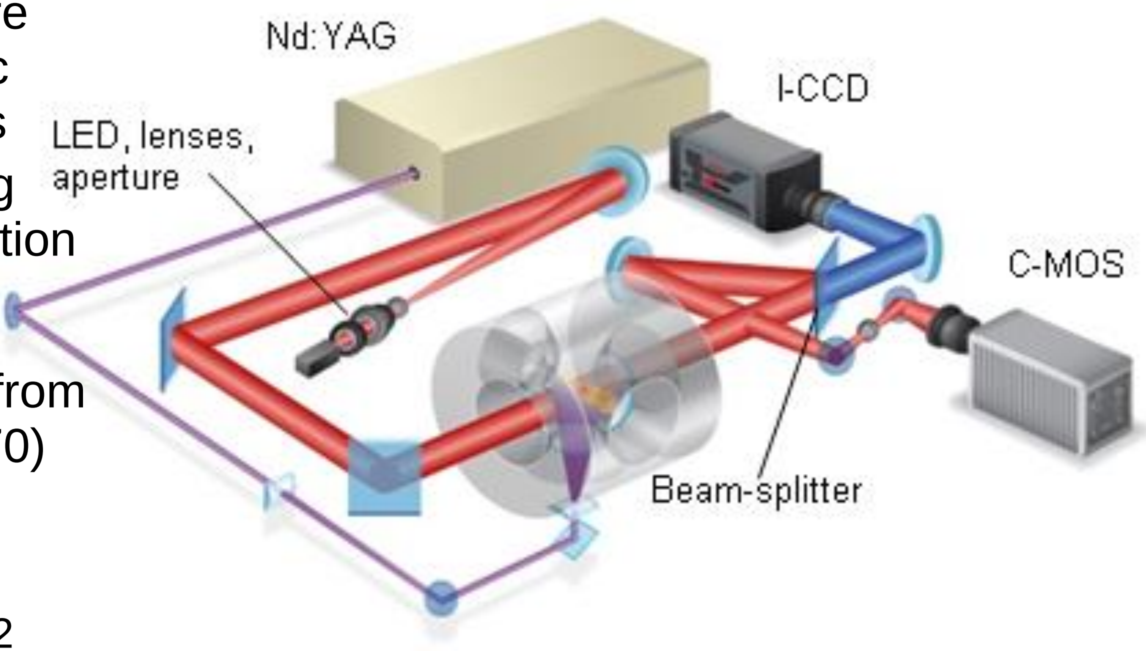
Imaging showed role of cool-flame-chemistry in high-pressure spray ignition (Skeen *et al*., Proc. Combust. Inst., 2015; Skeen *et al*., SAE Int. J. Engines, 2015)

- Initiation of low-temperature reactions near radial spray periphery
- Rapid appearance of cool-flame across entire spray head prior to ignition
- Volumetric 2nd stage ignition throughout broad equivalence ratio range

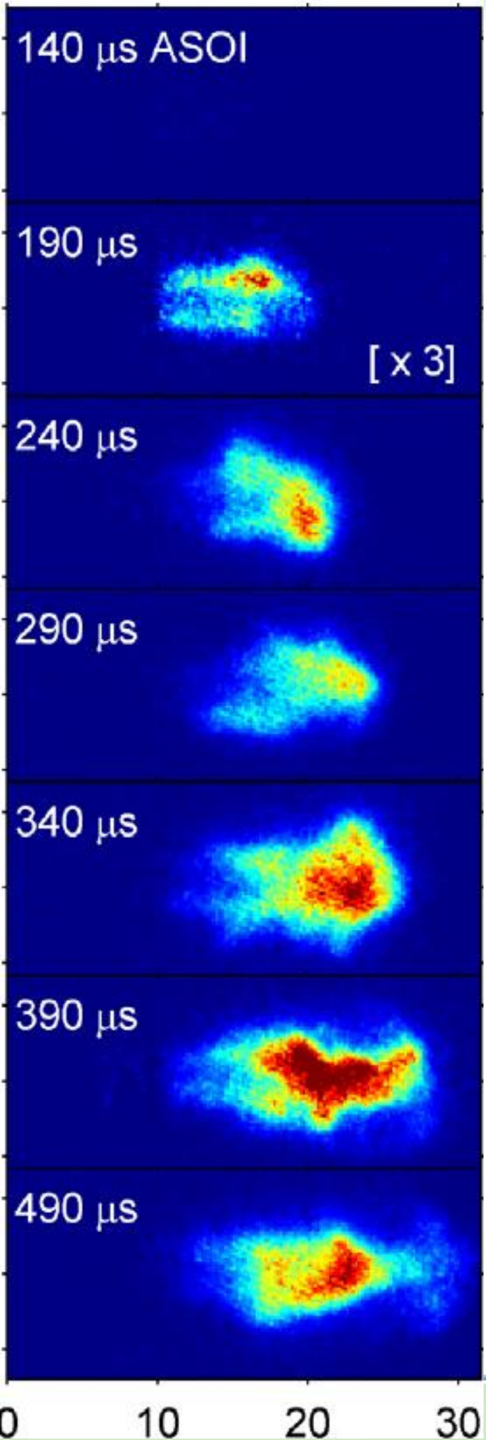
Simultaneous CH_2O PLIF & high-speed schlieren imaging provide key insight into ignition process

Scott A. Skeen & Lyle M. Pickett (Sandia-CRF)

- High-pressure, high-temperature vessel reaching thermodynamic condition relevant to CI engines
- Large optical windows providing multiple views of spray combustion event

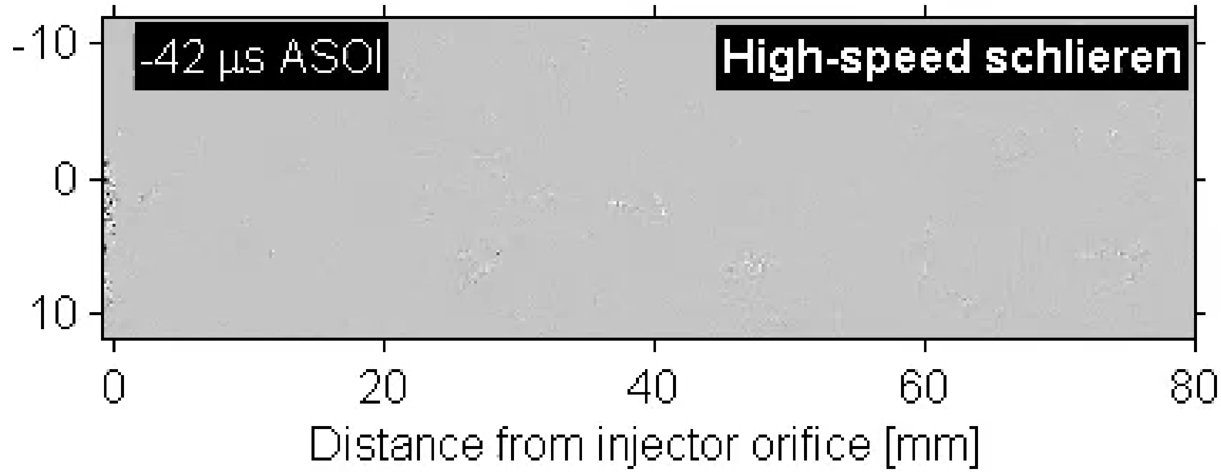


- Single-hole Bosch fuel injector from family of ECN injectors (s/n #370)
  - Injection pressure: 150 MPa
  - Fuel: n-dodecane ($C_{12}H_{26}$)
  - Chamber: 60 bar, 900 K, 21% O2
- High-speed (150 kHz) schlieren imaging
  - Cool flame (low-temperature ignition)
  - High-temperature ignition
  - Vapor penetration
- Single-shot formaldehyde (and PAH) PLIF with 355-nm (100-mJ/pulse) excitation
  - Select timings for multiple identical injection events



Formaldehyde & schlieren imaging show progression of ignition

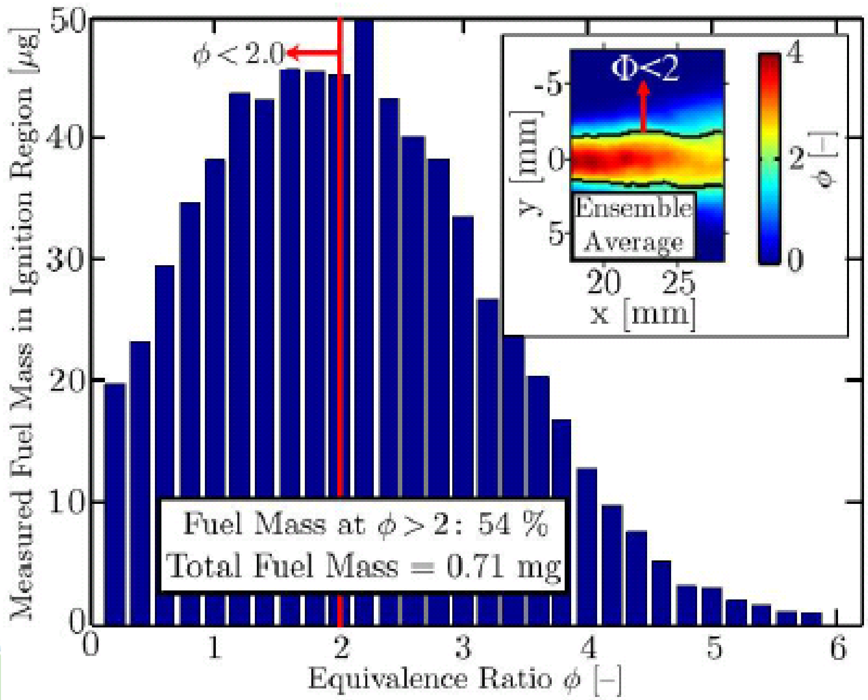
Scott A. Skeen & Lyle M. Pickett (Sandia-CRF)



- Initial cool-flame activity appears ≈200 μs ASOI in radial jet periphery
- Then, cool-flame rapidly appears throughout entire spray head within Δt≈200 μs **prior** to 2^{nd}-stage ignition
- This sequence of events is amazingly repeatable!

High-speed Rayleigh-Imaging: Fundamental relations in high-pressure sprays

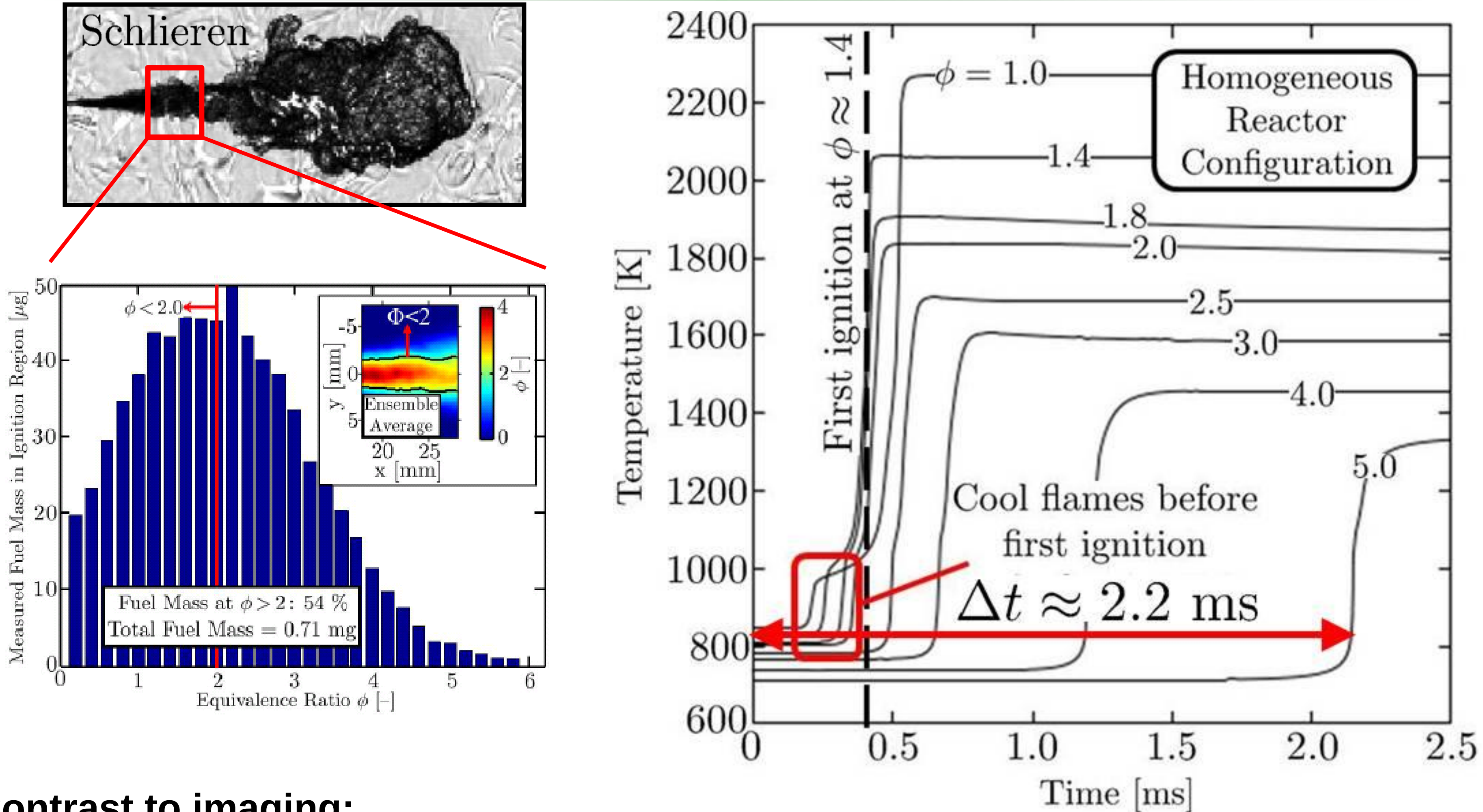
Scott A. Skeen & Lyle M. Pickett (Sandia-CRF)



High-speed Rayleigh:

- Lean & hot mixture in radial periphery of the jet
- Fuel-rich (ϕ≈5) & colder mixture in core region

Detailed kinetics-HR simulations (full LLNL) lead to fundamental inconsistency with experiments

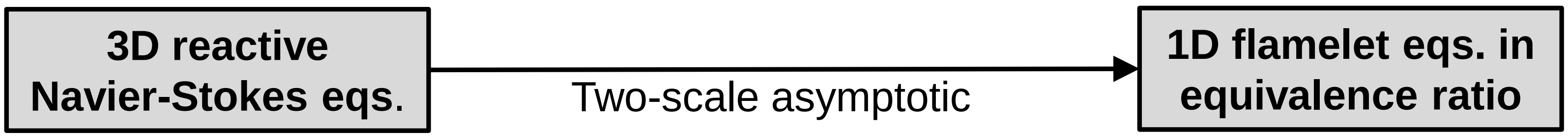


Contrast to imaging:

LLNL kinetics-HR simulations suggests cool flames only over (ϕ<1.4) until hot ignition

First-principles analysis of turbulent ignition

High turbulence, high-pressure, complex kinetics, large domains and time span
→ Revisiting Peters' derivation for burning flamelets (1984, 2000)
(All time and diffusion length scales & chemical pathways via LLNL kinetics)



True solution (!) of Navier-Stokes eqs. while asymptotic is valid → $Da = t_D / t_c >> 1$

- **Assumptions: (a) Binary fuel-oxidizer-system, (b) high scalar dissipation rates & (c) mixture fraction is determining quantity**

First-principles analysis of turbulent ignition

High turbulence, high-pressure, complex kinetics, large domains and time span
→ Revisiting Peters' derivation for burning flamelets (1984, 2000)
(All time and diffusion length scales & chemical pathways via LLNL kinetics)

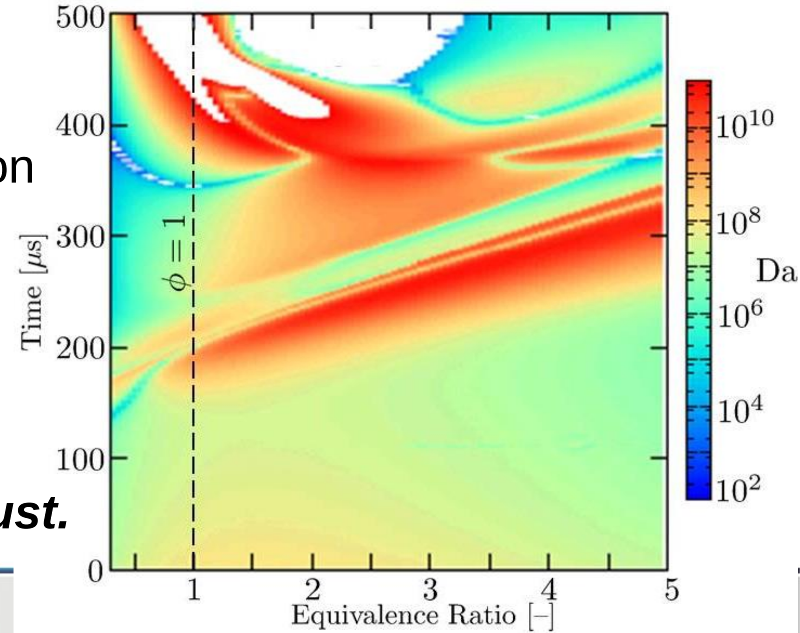
3D reactive Navier-Stokes eqs. → Two-scale asymptotic → **1D flamelet eqs. in equivalence ratio**

True solution (!) of Navier-Stokes eqs. while asymptotic is valid → Da=t_D/t_c>>1

- Chemical time scales t_c from CEMA
  (Law *et al.*, *JFM*, 2010)
- Diffusion time scales from instantaneous solution

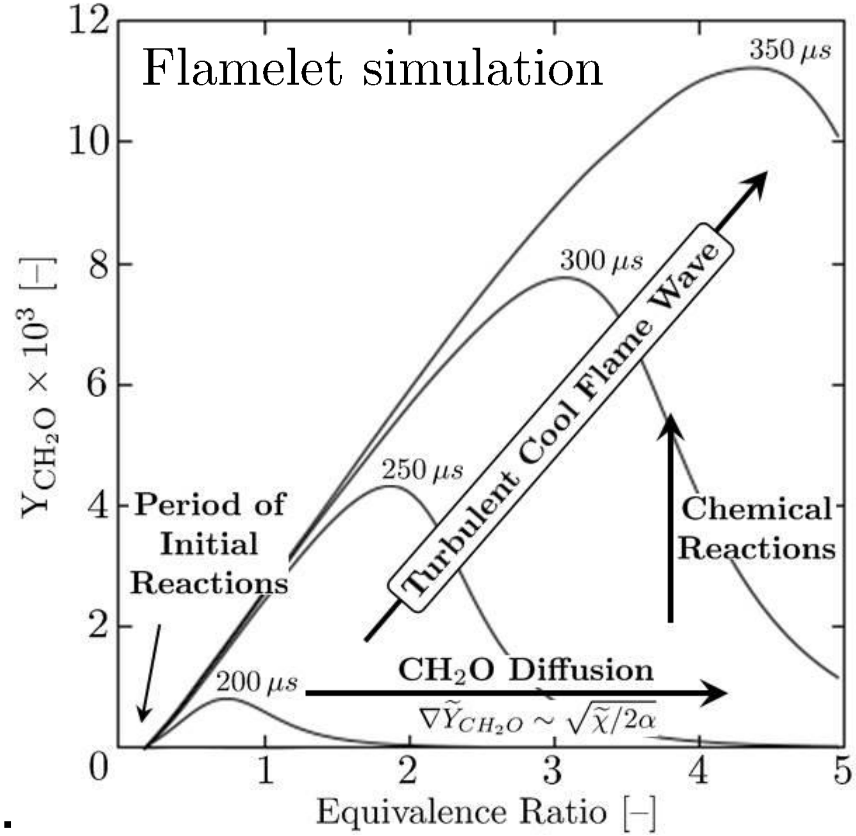
$$t_{D,i}^{-1} = \frac{1}{Y_{i,0}^2}\frac{\chi}{2}\left(\frac{\partial^2 Y_i}{\partial Z^2}\right)^2$$

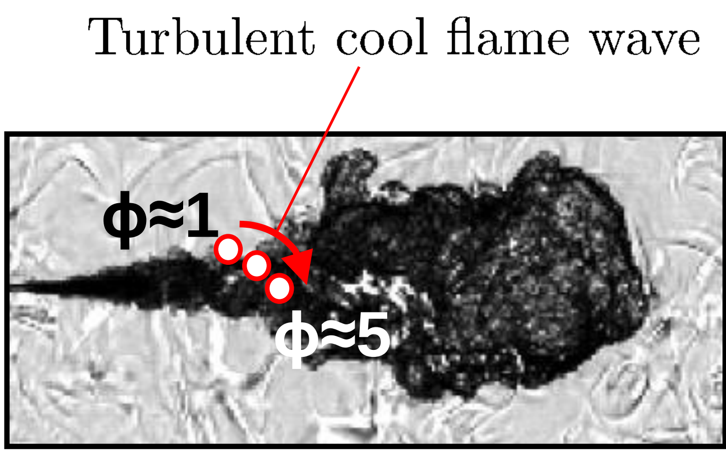
- Complete LLNL kinetics for n-dodecane
  (2755 species; 11,173 reactions)
- ***Asymptotic valid for low-temperature combust.***



Ignition mechanism of high-pressure spray flames
Turbulent flame configuration

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





Conclusion:

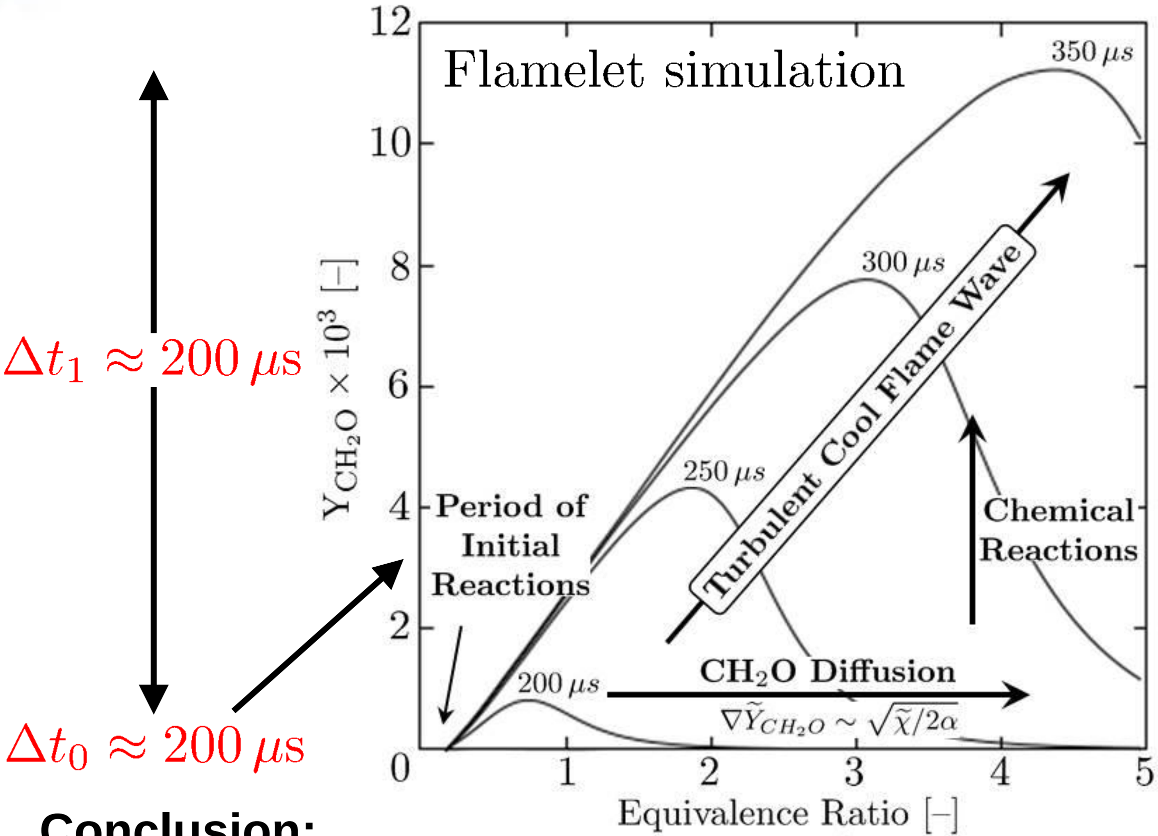
a) Species & temperature diffusion into neighbored mixture triggers 1st-stage ignition

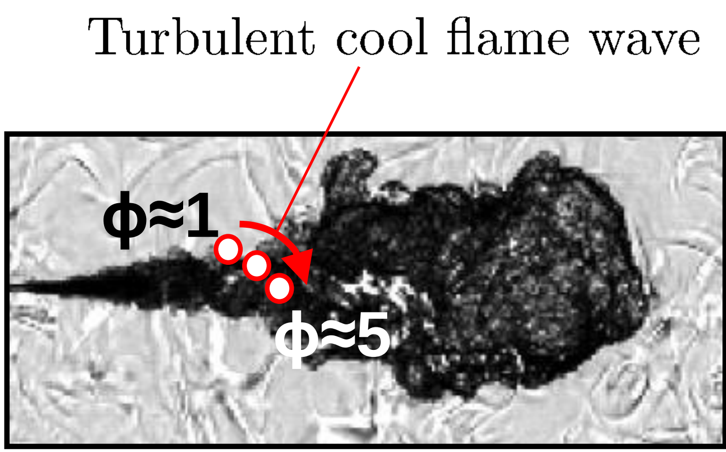
b) Continuous reactions & diffusion leads to cool flame wave propagation

Ignition mechanism of high-pressure spray flames

Turbulent flame configuration

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



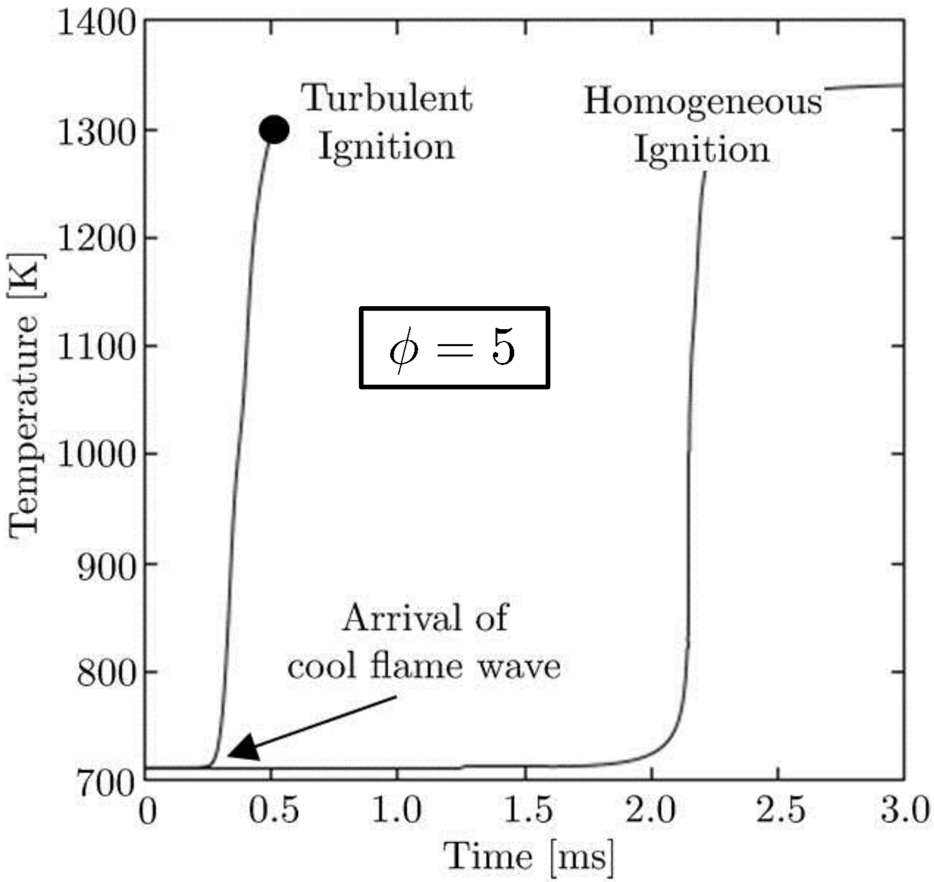


<u>Conclusion</u>:

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

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

Ignition mechanism of high-pressure spray flames



→ Turbulent cool flame wave significantly shortens ignition delay in rich mixtures
→ At ϕ=5, ignition delay decreases from 2.2 ms to 0.37 ms!
→ After hot ignition: Hot flame wave running back through pre-ignited mixture

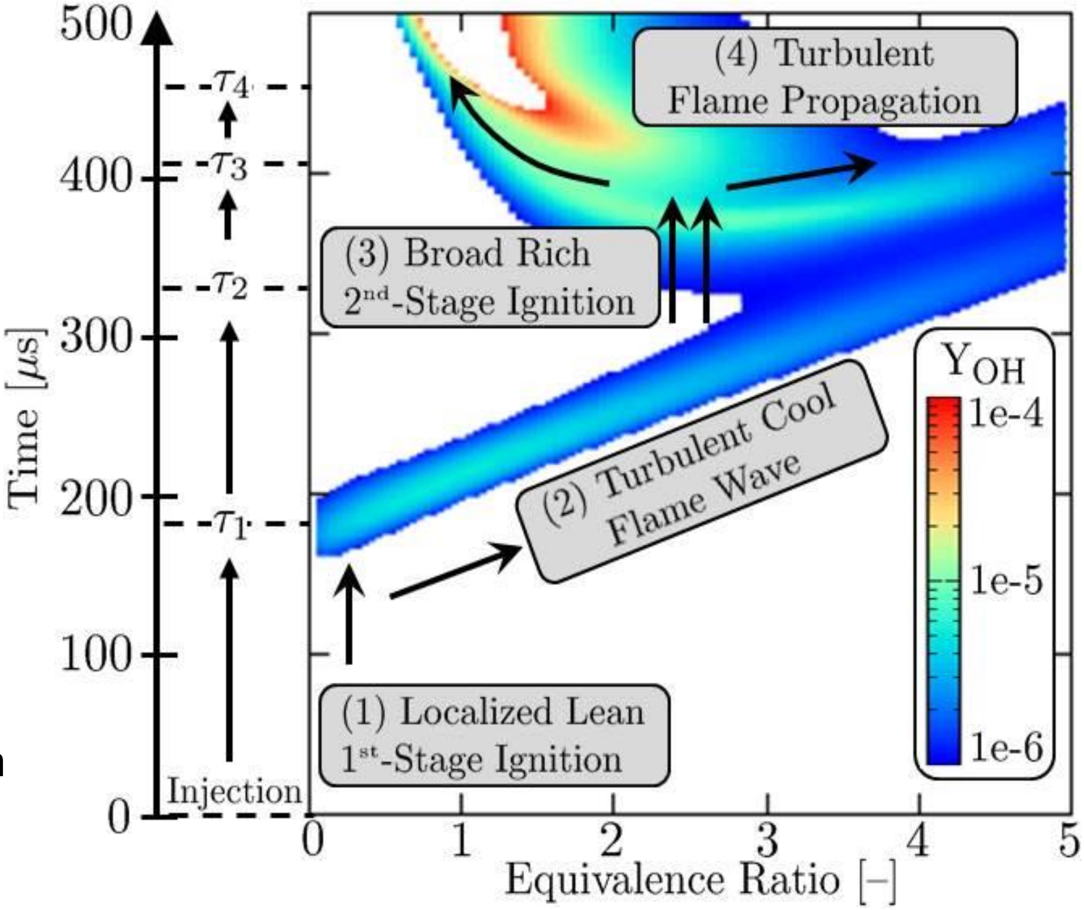
Imaging & simulations: Characteristic time scales in high-pressure spray flame ignition

1. t_1 (~200 µs):
   Initial period of chemical activity with first ignition in hot lean mixture

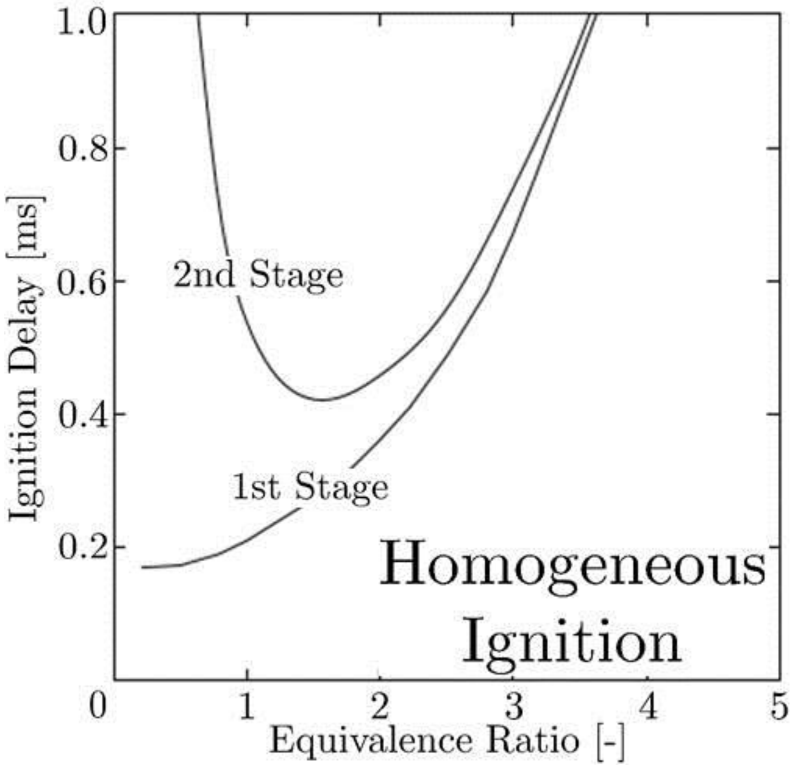
2. t_2 (~200 µs):
   Turbulent cool flame wave leads to cool-flame ignition of entire mixture

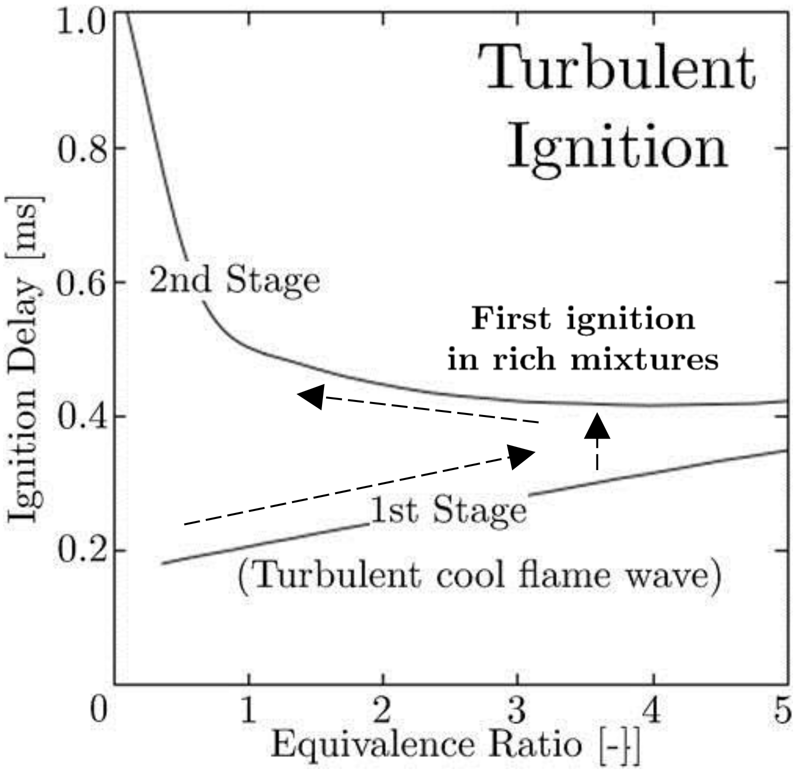
3. t_3 (~50 µs):
   Localized hot ignition in rich mixture where delay between 1st and 2nd stage of ignition is minimal

4. t_4 (~30 µs):
   Auto-igniting flame front propagation



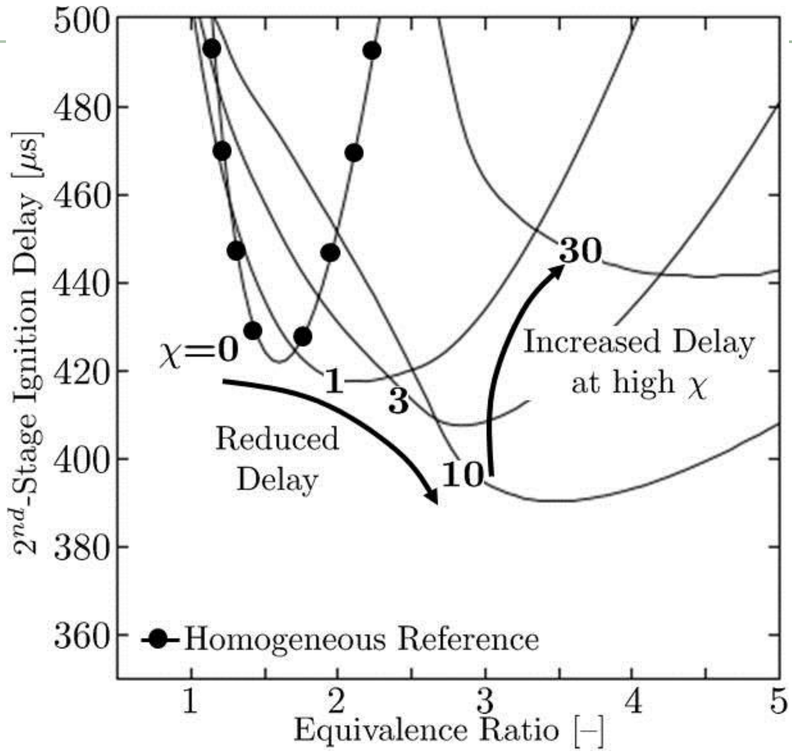
Ignition mechanism of high-pressure spray flames





→ Turbulent ignition waves lead to deviations from homogeneous ignition delays
→ Homogeneous settings (shock tubes etc.) deprived of this fundamental complexity

Mechanism of turbulent ignition resilient to fluctuations in scalar dissipation



→ Turbulent ignition delay decreases at first by increasing scalar dissipation
→ Then, ignition delay retards with further increase of scalar dissipation
→ But temporal evolution of turbulent ignition largely independent of turbulence level

Results published in R.N. Dahms, G.A. Paczko, S.A. Skeen, and L.M. Pickett, *Proc. Combust. Inst*. **36** (2016). In press. DOI: 10.1016/j.proci.2016.08.023

Summary and conclusions

- Prior imaging demonstrated significance of cool-flames in high-pressure spray flame ignition
- Neglect of turbulence (manifested as molecular diffusion) fundamentally fails to reproduce imaged physical processes of rich cool-flames before hot ignition
- Flamelet derivation shown to also hold during cool-flame ignition
- Simulation: Molecular transport results in rapidly propagating cool-flame waves which chemically activates entire mixture
- Hot ignition then occurs in rich mixture where the delay between 1st and 2nd stage of ignition becomes minimal
- Then, molecular transport & auto-ignition leads to propagating auto-igniting flame front
- Characteristic time scales of fundamental physical processes were consistent between experiments and simulation
- Fundamental mechanism of ignition is largely independent of intensity of scalar dissipation

Thank you for your attention!

The role of turbulence and cool-flame kinetics in high-pressure spray ignition

Rainer N. Dahms[1], Günter A. Paczko[2], Scott A. Skeen[1], and Lyle M. Pickett[1]

[1]*Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA*

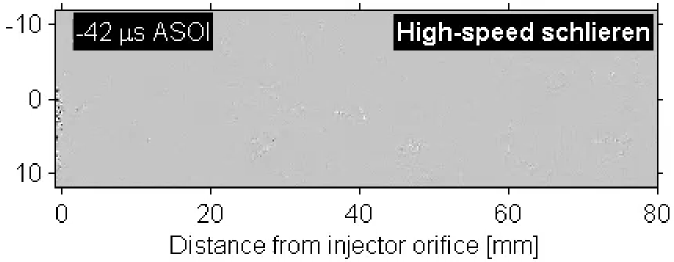
[2]*Institute for Combustion Technology, RWTH Aachen University, Germany*

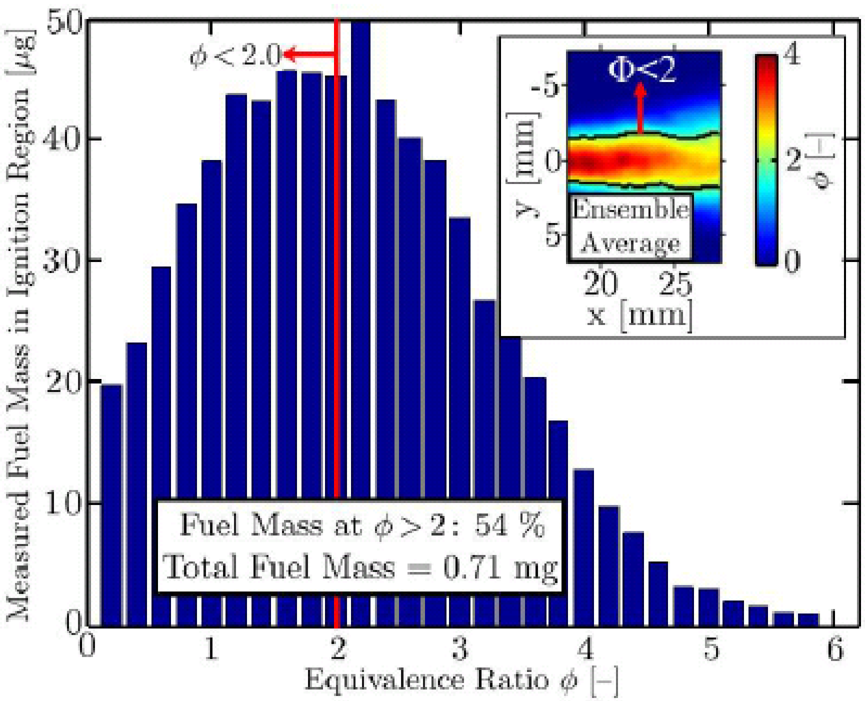
U.S. DEPARTMENT OF ENERGY | Office of Science | Energy Efficiency & Renewable Energy

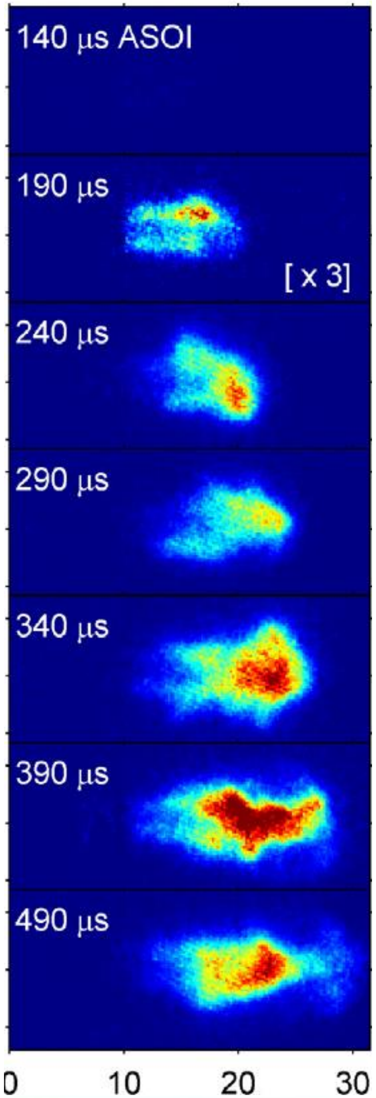
VEHICLE TECHNOLOGIES OFFICE

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences and Office of Vehicle Technologies

Fundamental relations in high-pressure Spray "A" flame



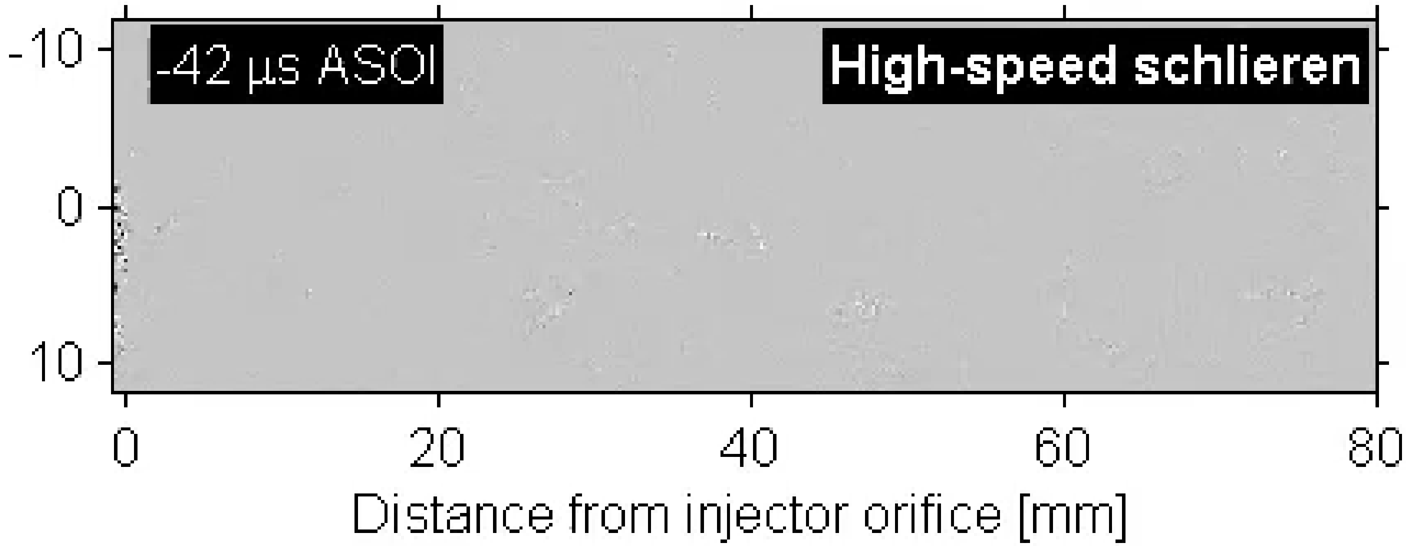




Formaldehyde imaging: Cool-flame ignition occurs over entire spray head (0<ϕ<5) within Δt≈200 μs after first appearance & before hot ignition

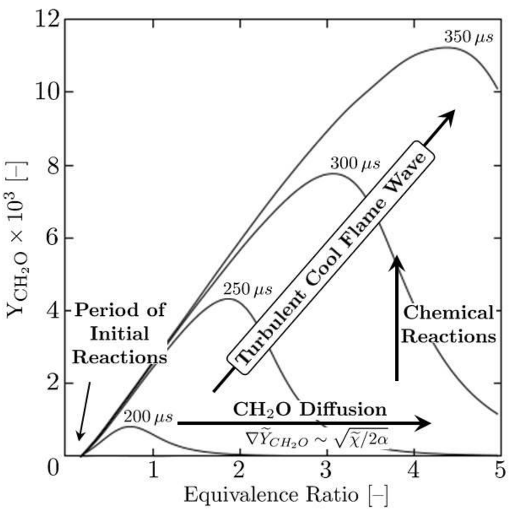
High-speed schlieren imaging yields spatial progression in 2-stage spray ignition

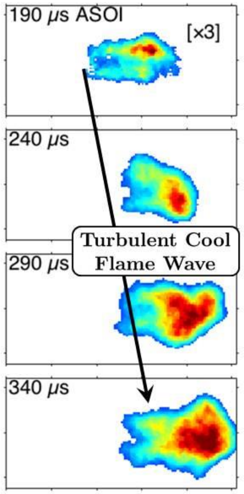
Scott A. Skeen & Lyle M. Pickett (Sandia-CRF)



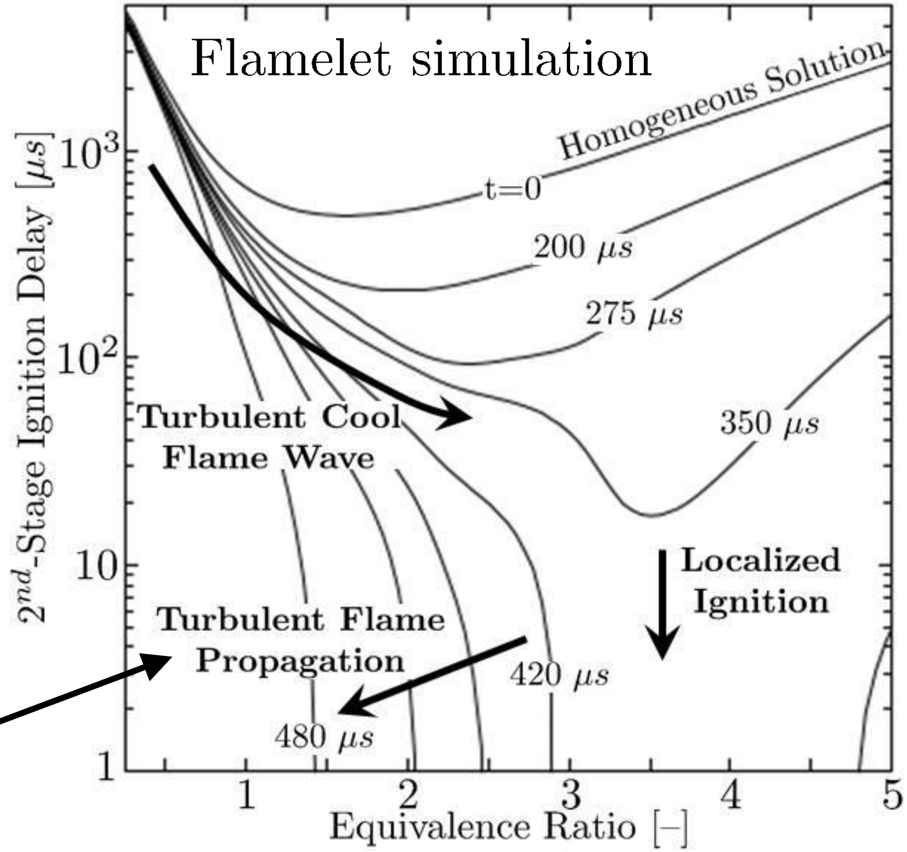
- Initial cool-flame activity appears ≈200 μs ASOI in radial jet periphery
- Then, cool-flame rapidly appears throughout entire spray head prior to second stage, high-temperature ignition
- This sequence of events is amazingly repeatable!

Ignition mechanism of high-pressure spray flames
Turbulent flame configuration





$\Delta t_3 \approx 50\,\mu s$



<u>Conclusion</u>:

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

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