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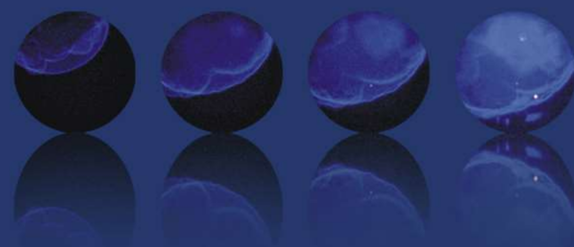
Wednesday, November 2nd , 2016



Fundamental Studies to Enable Robust, Reliable, Low Emission Gas Turbine Combustion of High Hydrogen Content Fuels: experimental and computational studies

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Acknowledgements

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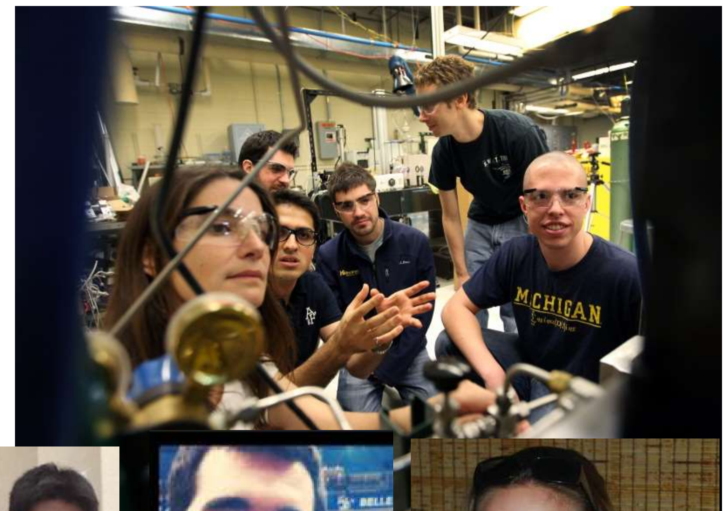
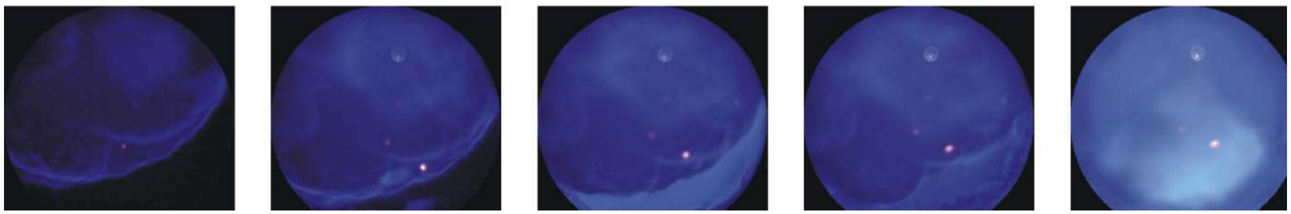


Many thanks to our UM team and the DOE NETL program!

outline



- *Program objectives*
- *Highlights of experimental results*
- *Highlights of computational results*

Program objectives

The proposed research program focuses on three areas to advance syngas turbine design:

1. syngas chemistry
2. fundamental ignition and extinction limits of syngas fuels
3. data distillation for rapid transfer of knowledge to gas turbine design.

The project objectives were:

1. To develop and validate accurate and rigorous experimental and computational data bases of syngas reaction kinetic and fundamental combustion properties,
2. To develop detailed and reduced syngas chemical mechanisms that accurately reproduce the new experimental data as well as data in the literature,
3. To develop a quantitative understanding of the stability of syngas combustion to fluctuations in the flow field, including the opportunities and challenges of exhaust gas recirculation (EGR) on extinction, ignition and flame stability,
4. To develop domain maps which identify the range of conditions (e.g. temperature stratification, turbulence, etc.) where syngas combustion can be effected in both positive and negative manners (e.g. accelerated autoignition).

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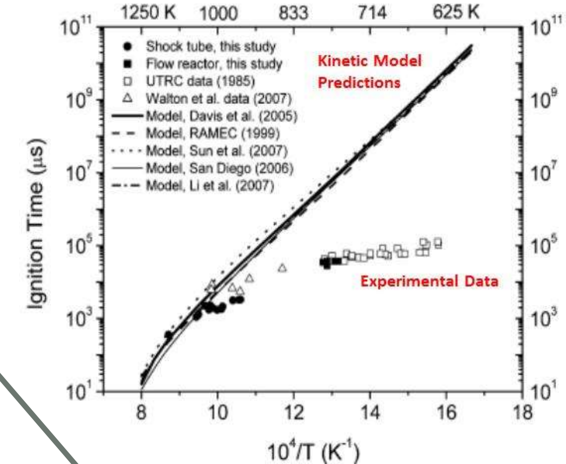
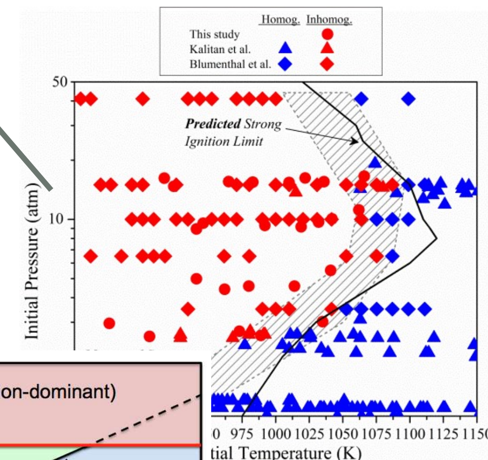
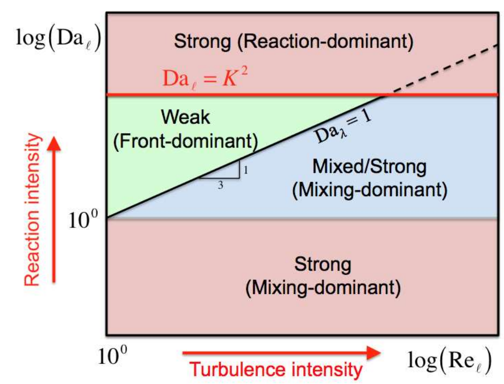
Chronology of outcomes

- Mansfield, A. B., Wooldridge, M. S., (2014) “High-pressure low-temperature **ignition behavior of syngas** mixtures,” *Combustion and Flame*, **161**, pp. 2242-2251.
- Mansfield, A. B., Wooldridge, M. S., Di, H., He, X., (2015) “Low-Temperature **Ignition Behavior of Iso-Octane** Mixtures,” *Fuel*, **139**, pp. 79-86.
- Im, H. G., Pal, P., Wooldridge, M. S., Mansfield, A. B. (2015) “**A Regime Diagram** for Autoignition of Homogeneous Reactant Mixtures with Turbulent Velocity and Temperature Fluctuations,” *Combustion Science and Technology*, **187**, pp. 1263-1275.
- Mansfield, A. B., Wooldridge, M. S., (2015) “The **Effect of Impurities** on Syngas Combustion,” *Combustion and Flame*, **162**, pp. 2286-2295.
- Pal, P., Mansfield, A. B., Wooldridge, M. S., Im, H. G., (2015) “A Computational Study of Syngas Auto-Ignition Characteristics at High-Pressure and Low-Temperature Conditions **with Thermal Inhomogeneities**,” *Combustion Theory and Modeling*, **19**, pp. 587-601.
- Pal, P., Valorani, M., Arias, P. G., Im, H. G., Wooldridge, M. S., Ciottoli, P. P., Galassi, R. M., (2016) “**Computational characterization of ignition regimes** in a syngas/air mixture with temperature fluctuations,” accepted for publication in the 36^{th} *Proceedings of the Combustion Institute*, July 2016.







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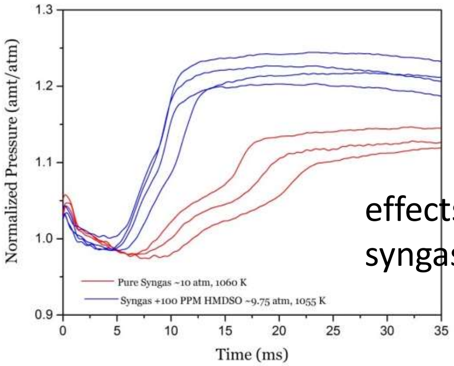
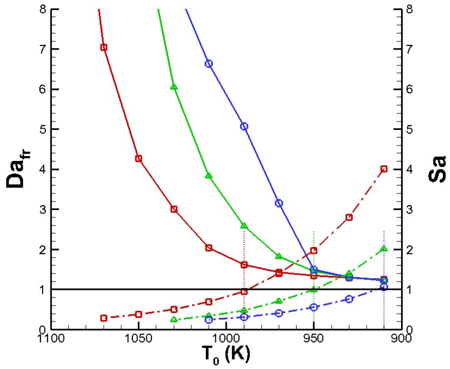
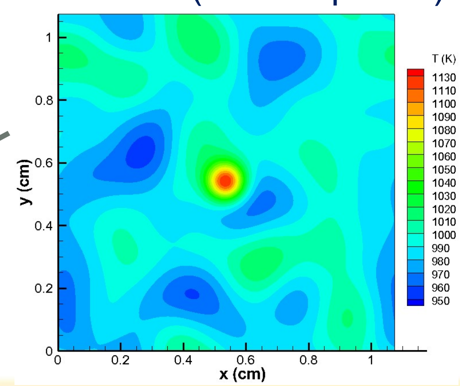


effects of HMDSO on syngas ignition



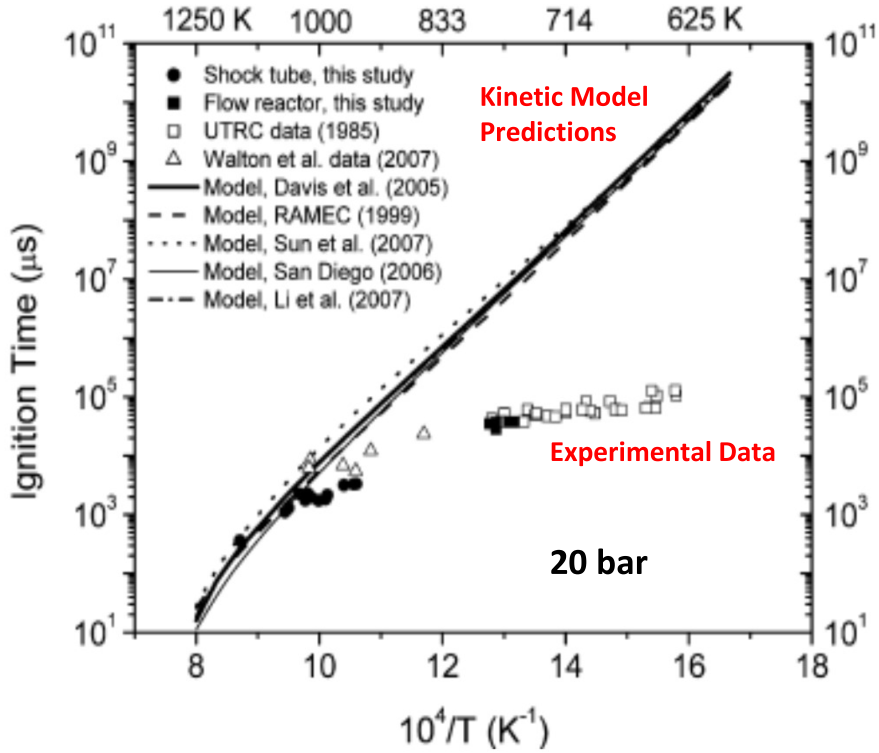
Case A (Initial T profile)



Motivation

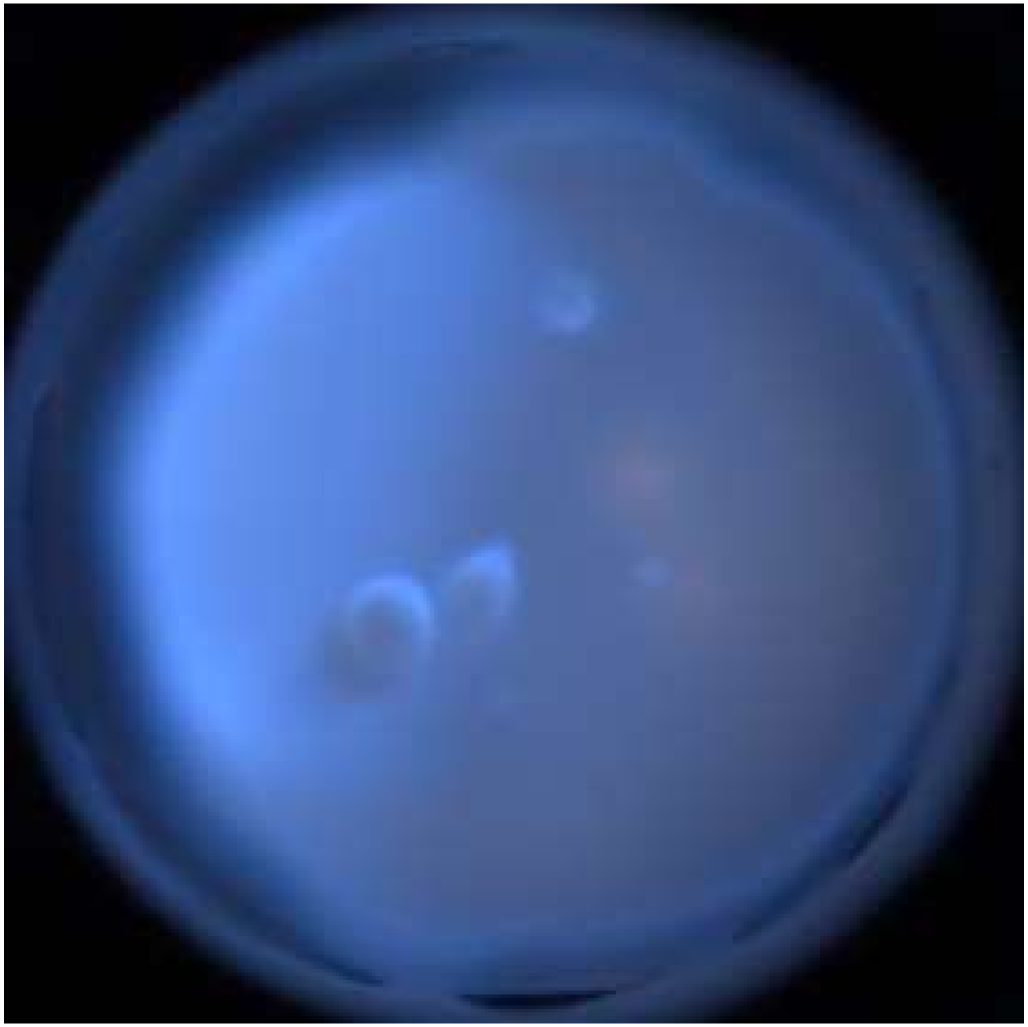
Why does ignition behavior matter?
What is the source of the observed discrepancies between models and experiments at lower temperatures?

- Ignition controlled by H_2/CO chemistry
- Ignition chemistry is relevant to flame chemistry
- Major discrepancy for low temperature syngas ignition delay
- Transition between weak and strong ignition could be the cause of observed discrepancies
- When does weak ignition occur and why? Possible explanations:
  - Uncertainties in rate coefficients
  - Incomplete reaction mechanisms
  - Surface-catalytic mechanisms
  - Wall heat transfer
  - Turbulence
  - **Ignition regimes**



Petersen et al.[3]

First color high-speed imaging of syngas ignition

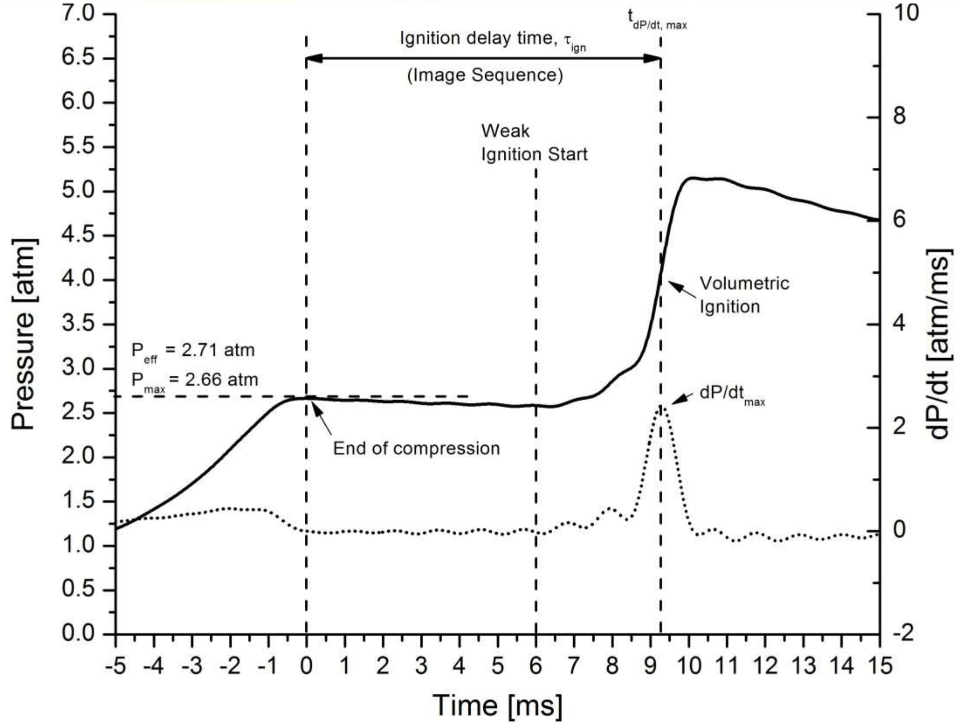


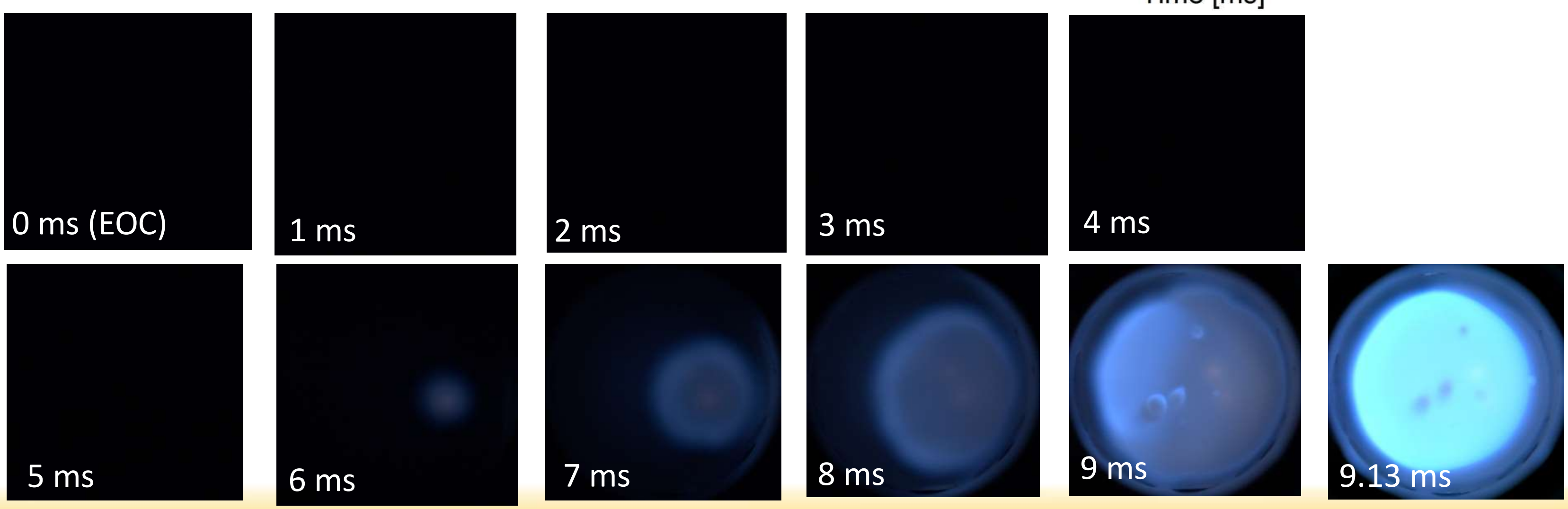
Defining weak, strong and mixed ignition.
← an example of mixed ignition

CMOS imaging, high-speed color digital video camera: 25,000 fps, 512× 512 pixels, exposure time of 40 μs

Typical results: mixed syngas ignition

- Pressure time history
- High-speed imaging
- T = 1006 K, P = 2.71 atm
- Inert gas: O_2 ratio = 5.91
- $\phi = 0.5$,
- 5.04% H_2, 7.26% CO





Experimental results for syngas isolate the source of discrepancy

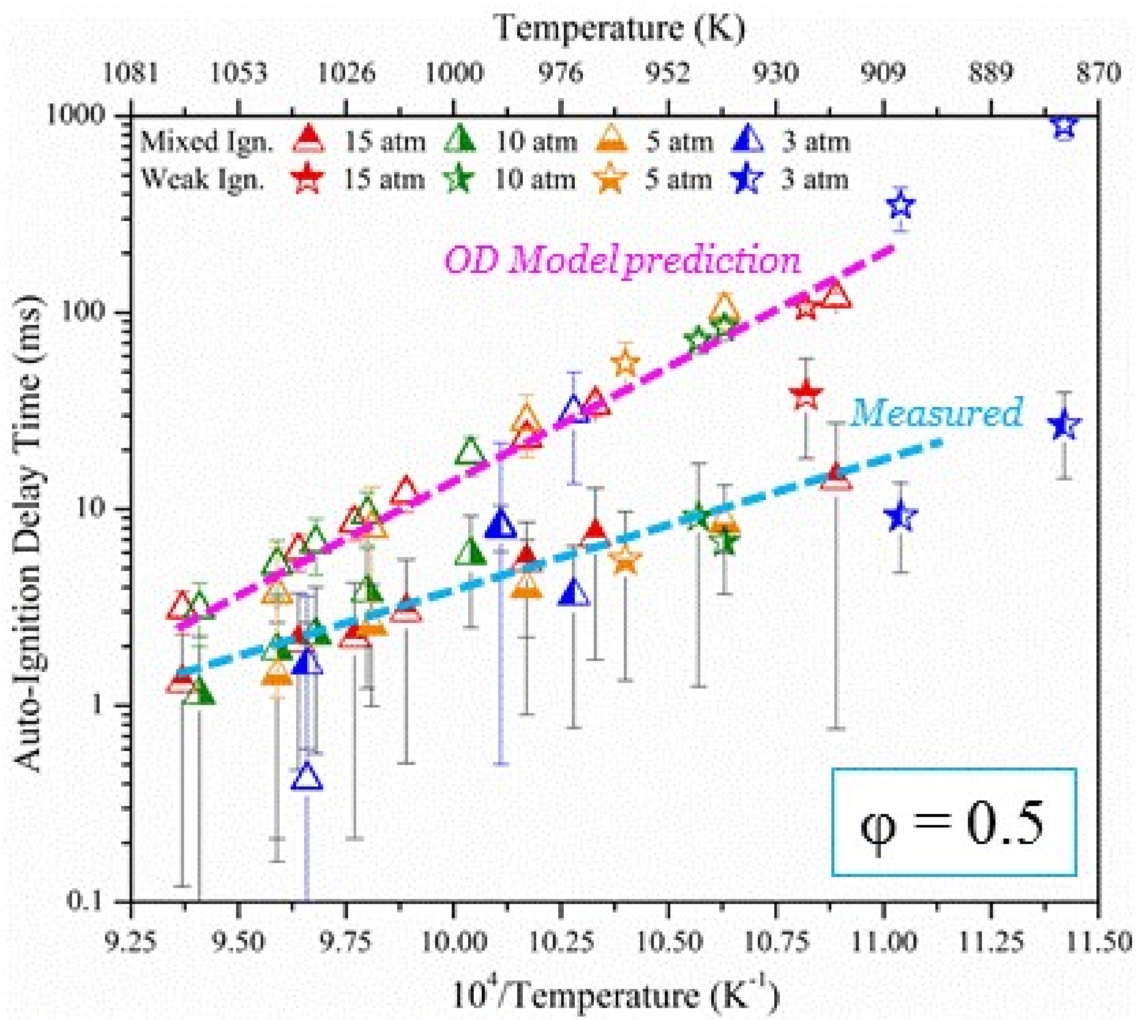
So we identify weak, strong and mixed ignition for a large state and syngas mixture composition space.

P = 3.3 atm, T = 1043 K, φ = 0.1

P = 9.2 atm, T = 1019 K, φ = 0.5

Experimental results for syngas isolate source of discrepancy

Weak ignition accelerates ignition delay times.
Larger effects observed at lower temperatures.



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Can we correlate syngas ignition behavior?

Yes! We can map P, T auto-ignition behavior of syngas mixtures. Invaluable for captains in uncharted territory, i.e. for data interpretation, to develop and test theory, to design stable systems, etc. But takes a lot of effort.

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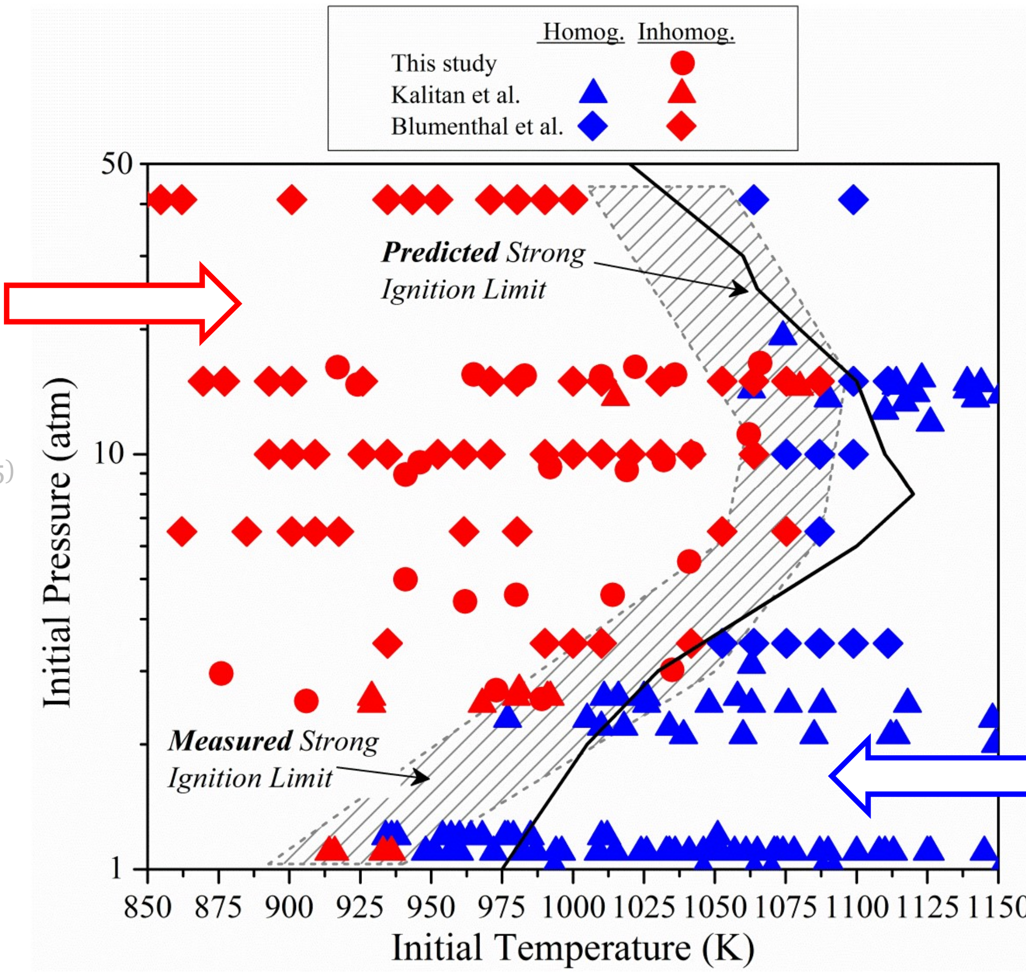
(P = 9.2 atm, T = 1019 K, φ = 0.5)

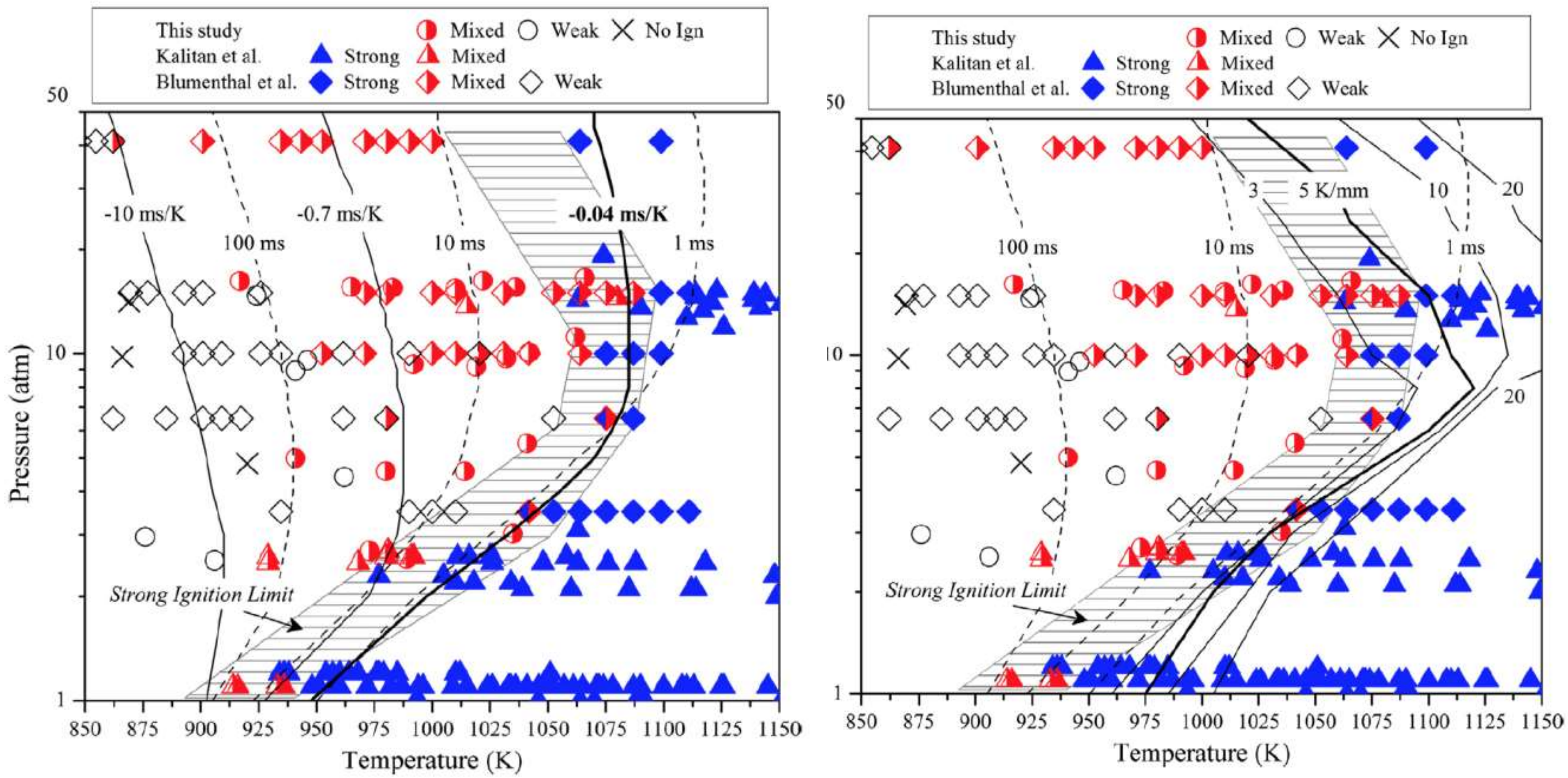


(P = 3.3 atm, T = 1043 K, φ = 0.1)

φ = 0.5,
Air Dil.

Can we predict syngas ignition regimes?

Yes! The boundary of ignition regimes can be predicted using $d\tau_{ign}/dT$ (fuel property) or dT/dx (state condition).



But what about other fuels, other conditions, turbulence, etc.?
Is there a unifying theory?

Yes! There is a unifying theory to predict ignition behavior

The Zeldovich(1980)-Sankaran(2005) ignition criterion **for laminar flame systems:**

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} = \beta S_L \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \left(\frac{dT}{dx} \right) \qquad \beta \approx 0.5$$

$$\begin{cases} \mathrm{Sa} > 1 & \text{Deflagration – Weak Ignition} \\ \mathrm{Sa} < 1 & \text{Spontaneous Front – Strong Ignition} \end{cases}$$

where $\beta < 1$ reflects the fact that very rapid spontaneous front propagation is needed to ensure nearly homogeneous strong ignition.

Validated with UM RCF syngas ignition experiments.
But what about the effects of turbulence?

Extending the laminar ignition regime criteria

We defined a turbulent Sankaran Number:

$$\mathrm{Sa} = K\mathrm{Da}_\ell^{-1/2}$$

where $K = \beta\left(\dfrac{T'}{\sqrt{\tau_{ig}\tau_f}}\right)\left(\dfrac{d\tau_{\mathrm{ig}}}{dT}\right)$ Non-dimensional ignition sensitivity

Ignition Criterion: $\begin{cases} \mathrm{Da}_\ell < K^2 & \text{Weak} \\ \mathrm{Da}_\ell > K^2 & \text{Strong (reaction-dominant)} \end{cases}$

However, the fluctuations will dissipate before the front forms if $\mathrm{Da}_{\lambda,\mathrm{ig}} < 1$

$$\mathrm{Da}_{\lambda,\mathrm{ig}} = \mathrm{Da}_\ell \mathrm{Re}_\ell^{-1/3} \qquad \begin{cases} \mathrm{Da}_{\lambda,\mathrm{ig}} > 1 & \text{Weak ignition possible} \\ \mathrm{Da}_{\lambda,\mathrm{ig}} < 1 & \text{Mixed/Strong (mixing-dominant)} \end{cases}$$

$\mathrm{Da}_\ell < 1$ Strong (mixing-dominant)

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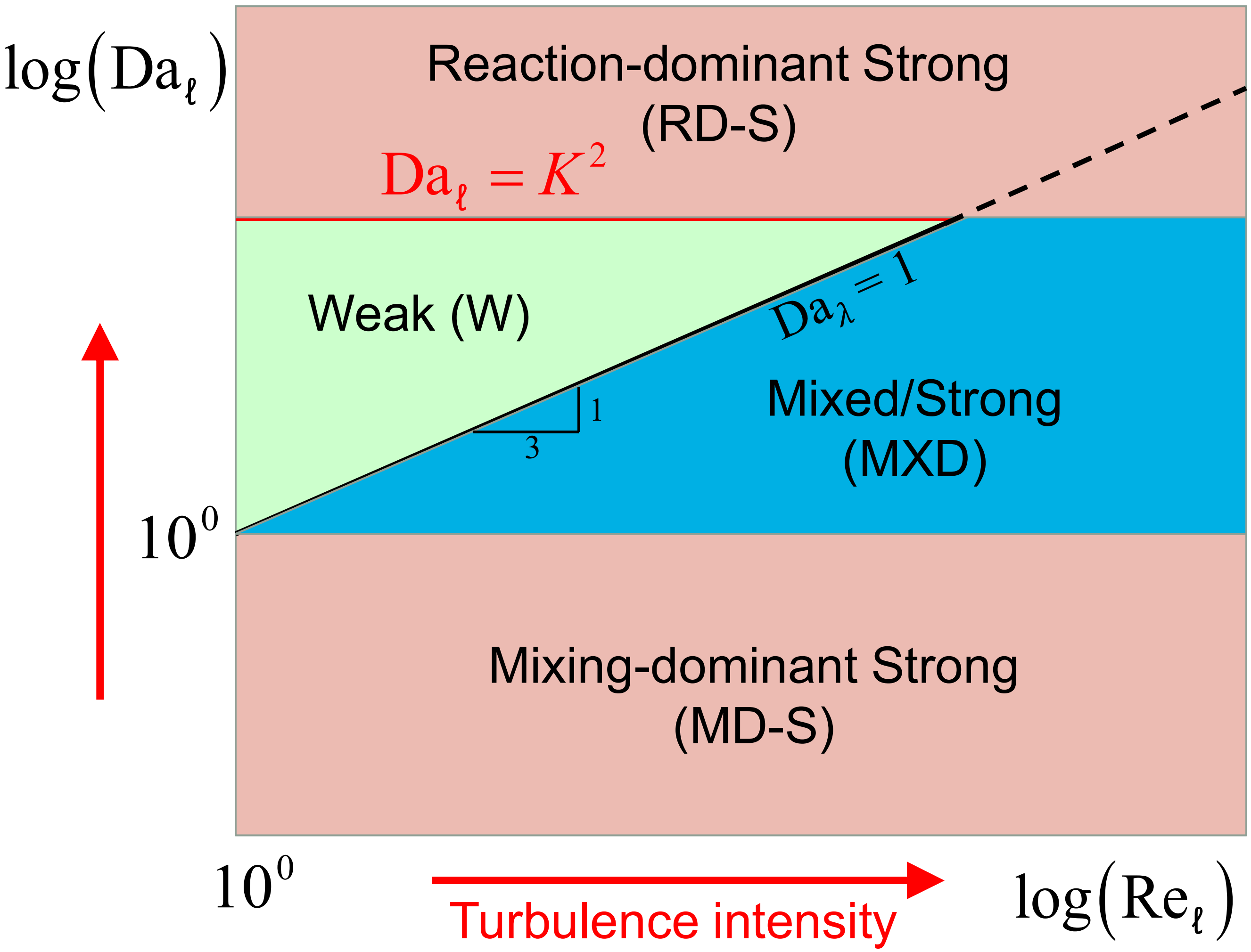
Turbulent Ignition Regime Diagram



integral eddy scale

$$Da_\ell = \frac{\tau_\ell}{\tau_{ig}} = \frac{\ell / u'}{\tau_{ig}}$$

Taylor micro scale

$$Da_\lambda = \frac{\tau_\lambda}{\tau_{ig}} = Da_\ell \, Re_\ell^{-1/3}$$

$$K = \beta \sqrt{\frac{\tau_f}{\tau_{ig}}} \left(\frac{T'}{\tau_f}\right) \left(\frac{d\tau_{ig}}{dT}\right)$$

Regime Diagram Validation

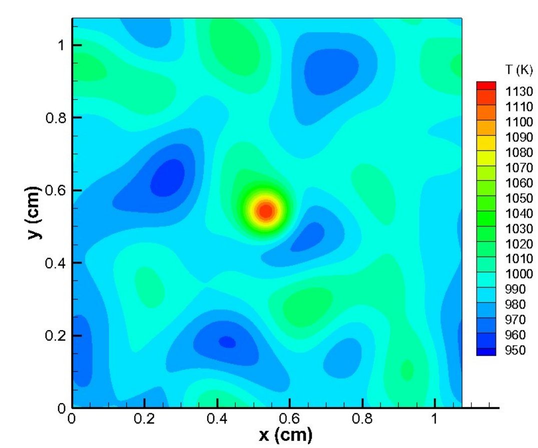
2D DNS of Syngas Autoignition: Numerical Setup

P_0 = 20 atm, φ = 0.5, H_2: CO = 0.7:1 (molar)

Case	T_0 (K)	τ_{ig} (ms)	K^2	ℓ_e (mm)	u' (m/s)	τ_t (ms)	Da_ℓ	Re_ℓ	Da_λ	Ignition Regime
A	990	25.8	4.05	4.3	0.05	86.0	3.34	35.3	1.02	W
B	1100	2.07	2.51	4.3	0.05	86.0	41.6	29.4	13.5	RD-S
C	990	25.8	4.05	4.3	1.5	2.87	0.11	1057	0.01	MD-S
D	1100	2.07	2.51	1.4	0.325	4.31	2.08	62.2	0.6	MXD
E	1020	12.7	3.28	4.0	0.3	13.33	1.05	185	0.2	MXD
F	1100	2.07	2.51	6.0	0.2	30.0	14.5	164	2.65	RD-S
G	990	25.8	4.05	6.0	0.2	30.0	1.16	197	0.2	MXD
H	970	41.3	4.41	6.0	0.05	120.0	2.91	50.0	0.8	MXD

- Periodic boundary conditions on all sides
- Passot-Pouquet turbulent kinetic energy spectrum
- Uncorrelated temperature and velocity fields
- Hot spot superimposed on the random T field at the center of the domain
- Syngas/air detailed chemical kinetic mechanism with 12 species and 33 reactions (*Li et al. 2007*)

Case A (Initial T profile)



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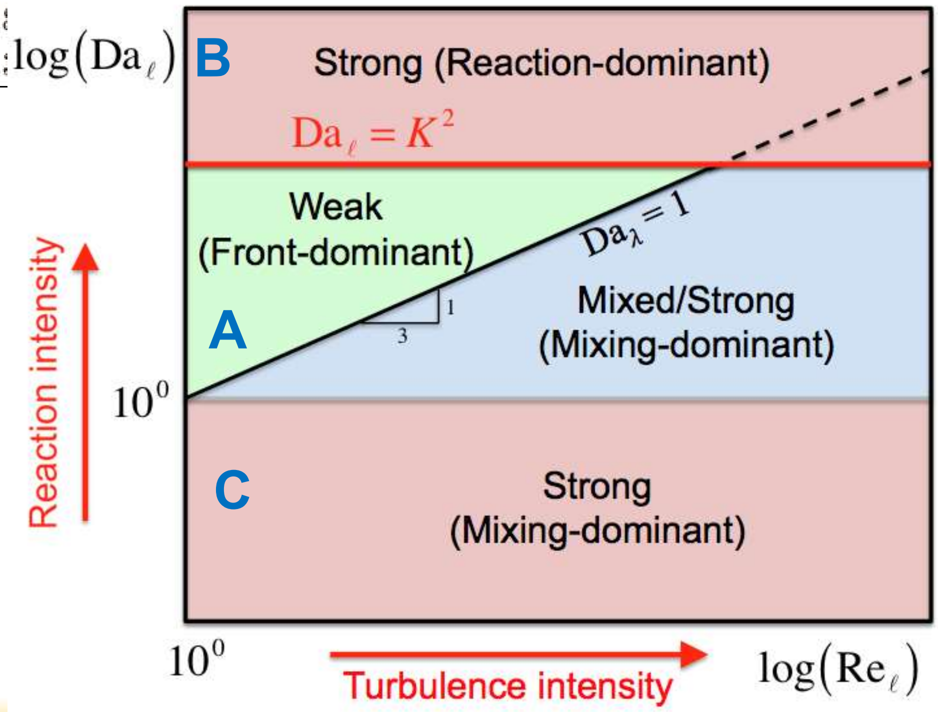
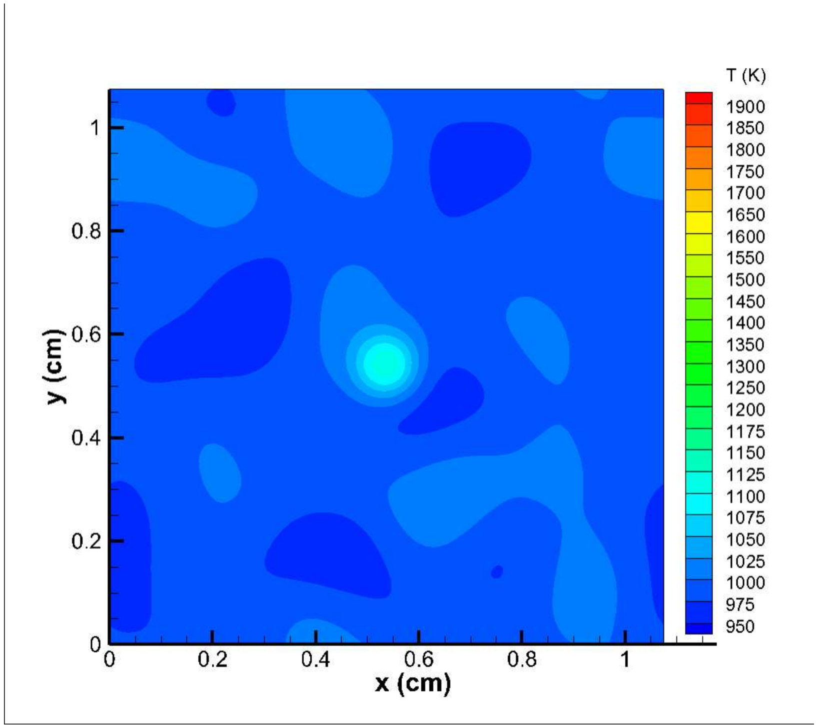
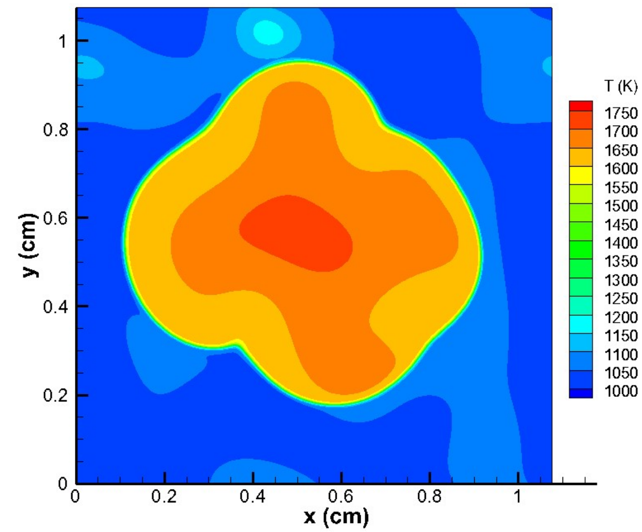
F	1100	2.07	2.51	6.0	0.2	30.0	14.5	164	2.65	RD-S
G	990	25.	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.97	0.2	MXD
H	970	41.	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0	0.8	MXD



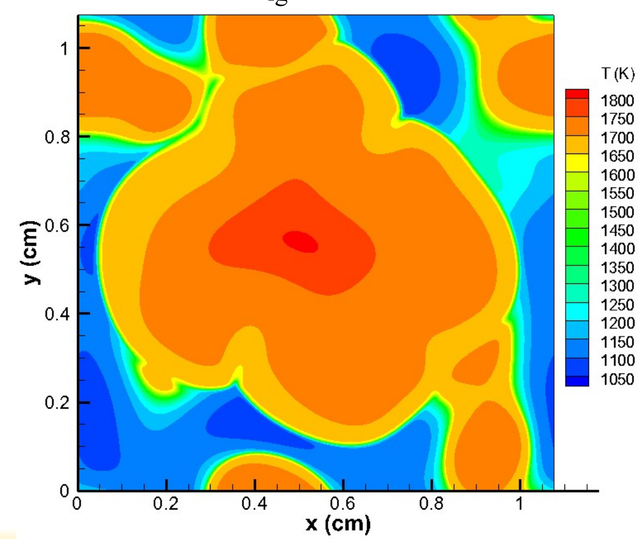
Case A: Weak Ignition



$t / \tau_{ig} = 0.41$

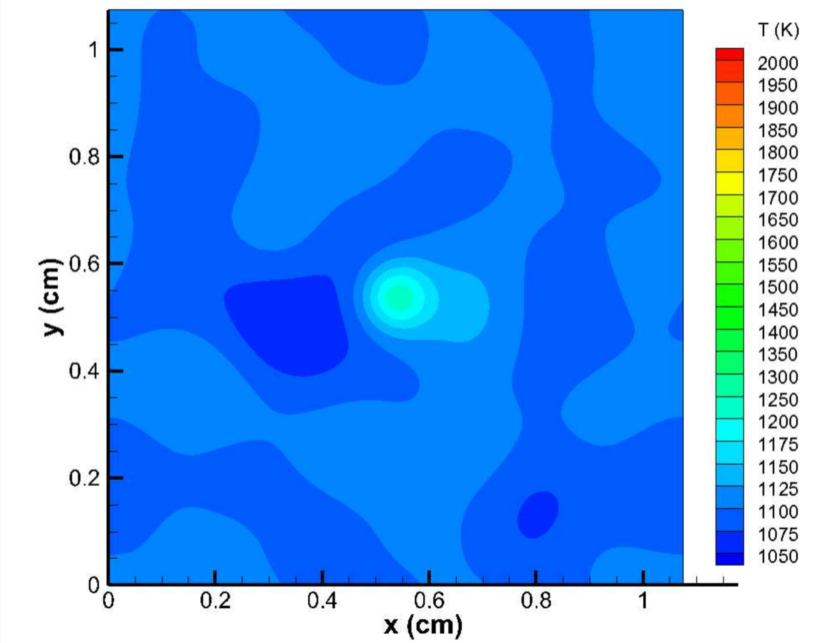


$t / \tau_{ig} = 0.48$

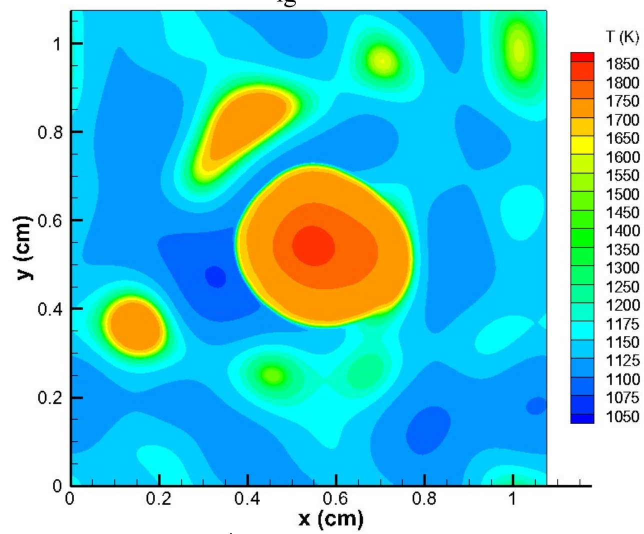


A reaction front consumes a significant portion of the mixture until the end-gas auto-ignition occurs.

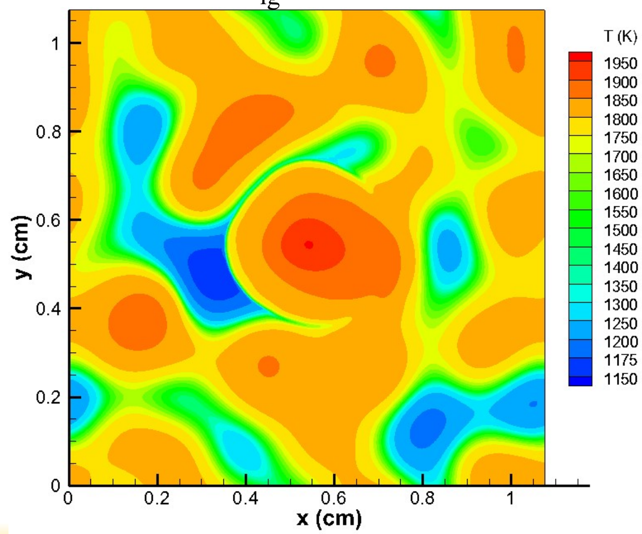
Case B: Strong Ignition - Reaction Dominant



$t / \tau_{ig} = 0.63$

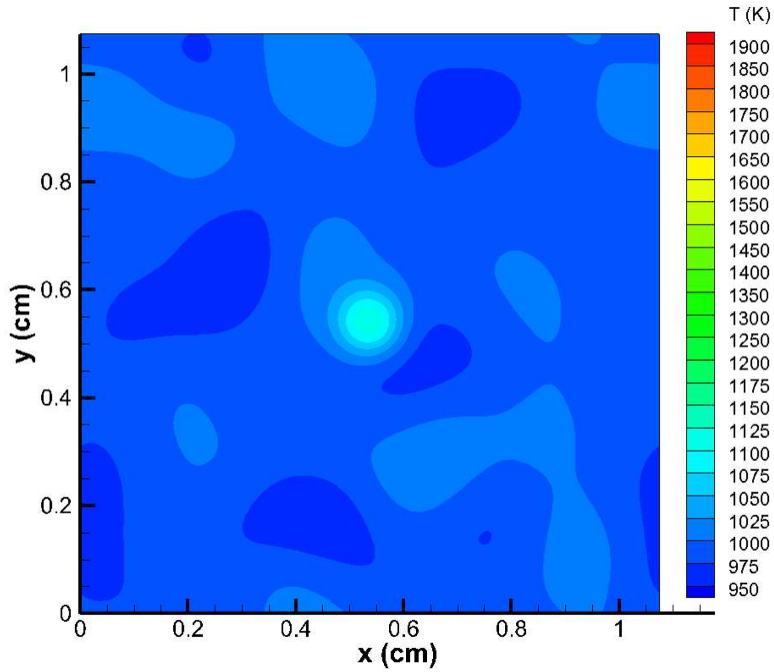


$t / \tau_{ig} = 0.77$

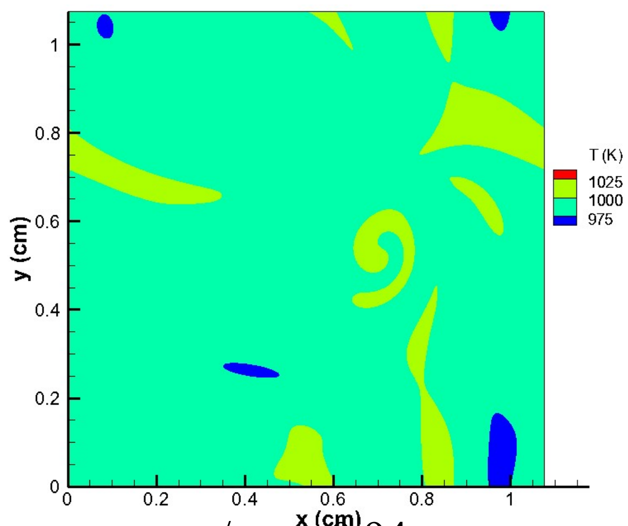


Due to the high reactivity and lower temperature sensitivity of the bulk mixture, the ignition kernel quickly leads to the bulk gas auto-ignition; spontaneous ignition front emanates from the ignition kernel.

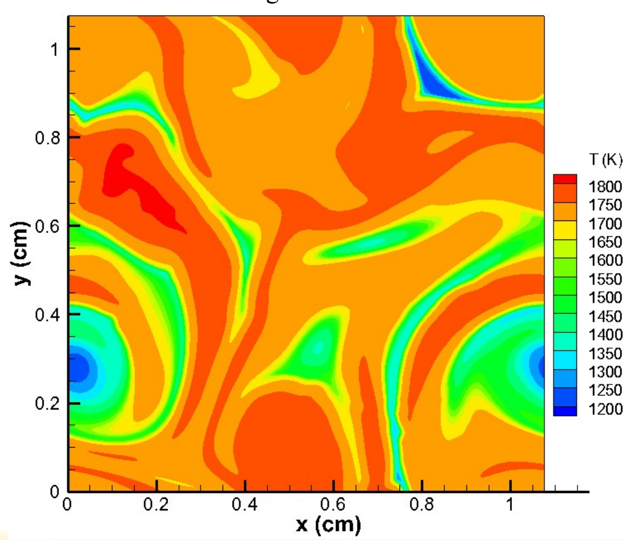
Case C (Strong Ignition – Mixing-Dominant)



$t / \tau_{ig} = 0.33$

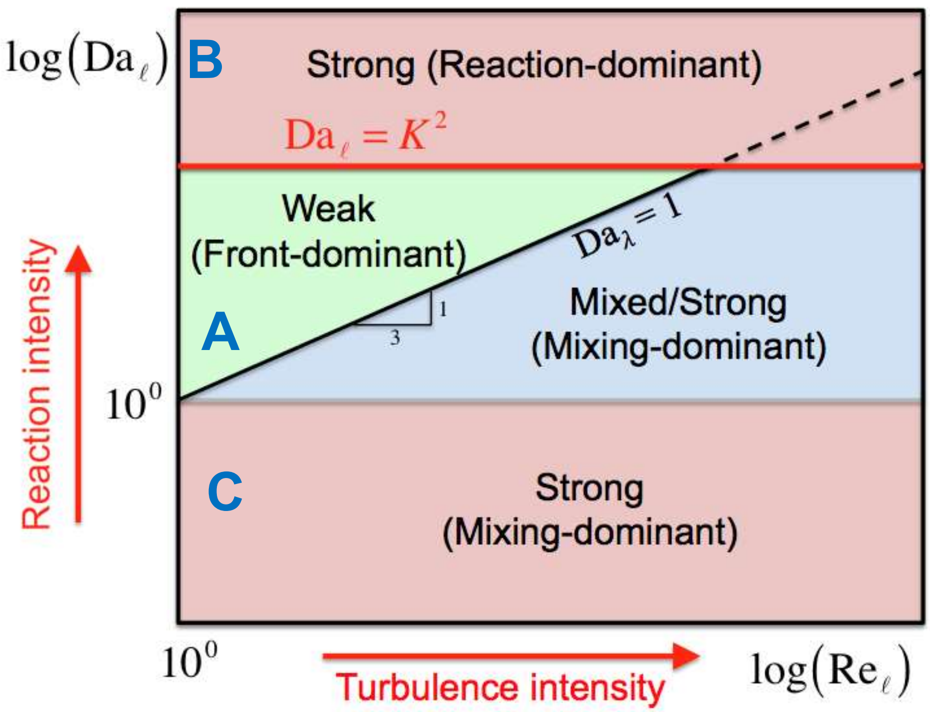


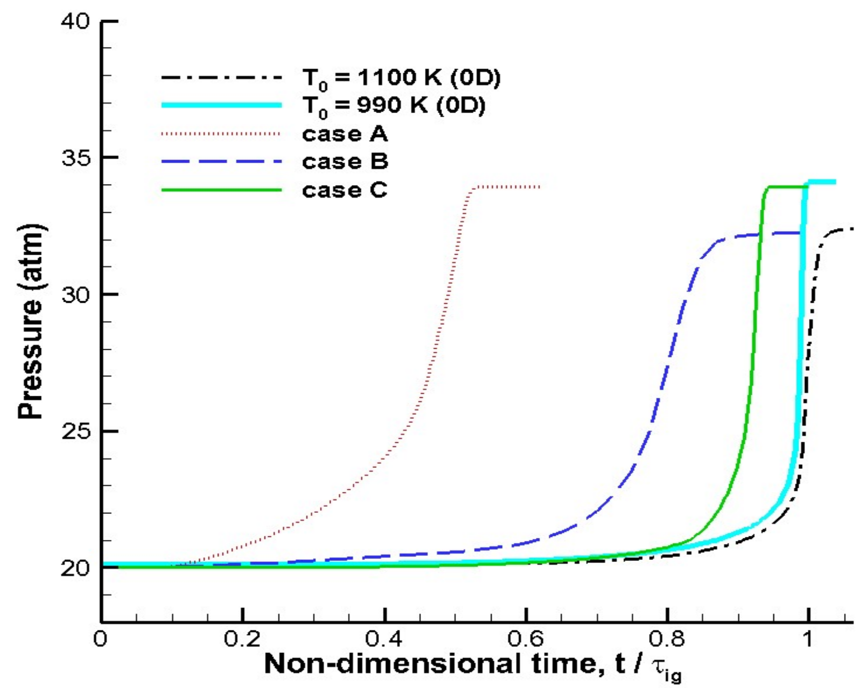
$t / \tau_{ig} = 0.94$



The stronger turbulence leads to rapid dissipation of the scalar fluctuations, resulting in nearly homogeneous auto-ignition.

Pressure Time Histories





Case A shows significant ignition enhancement compared with cases B and C! Weak ignition accelerates ignition in comparison to a homogeneous initial condition. ← Additional confirmation of the source of the modeling and experimental discrepancies.

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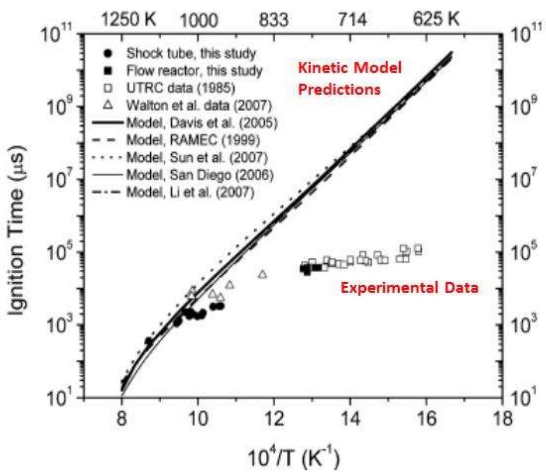
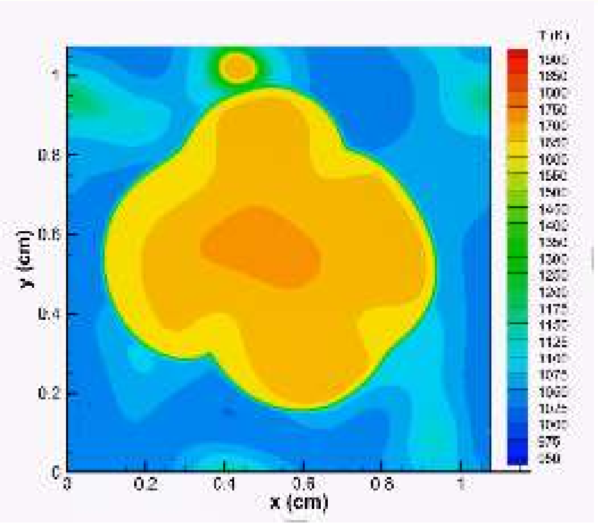
Summary and Reflections





Mystery solved/discrepancy resolved!

- The Zeldovich-Sankaran criterion predicts weak/strong ignition behavior in terms of global parameters.
- Theory has been validated by physical and numerical experiments.
- The ignition sensitivity (*K*) is more than just a characteristic time scale, a conventional Da-Re characterization is not sufficient to describe the ignition/combustion phenomena.
- High-*K* mixtures are more susceptible to weak ignition, which happens at low temperatures for hydrogen/syngas mixtures.
- *The observed ignition advancement for syngas at low temperatures can be attributed to weak ignition behavior.*

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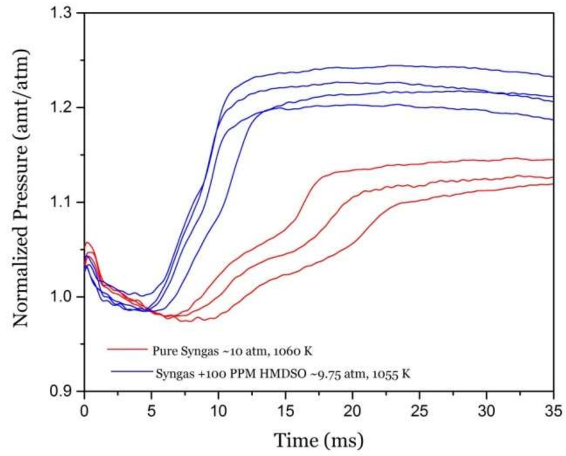
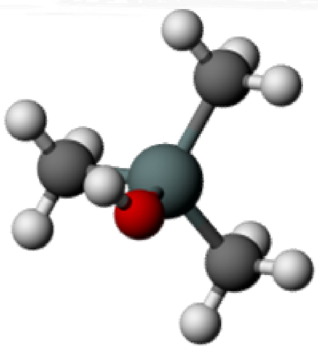
Wrapping-up our syngas studies

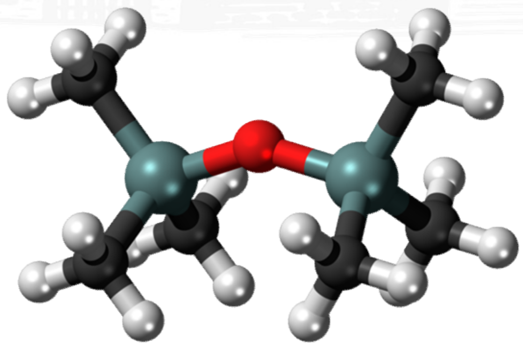
- Experimental studies of syngas OH kinetics and the effects of impurities on syngas combustion - particular concern for organosilicon compounds
- Silanols, siloxanes increasing in concentration in landfill-based syngas.
- Known to foul; effects on combustion?
- Studies of TMS and HMDSO completed
- OH data acquired and kinetic analysis in process





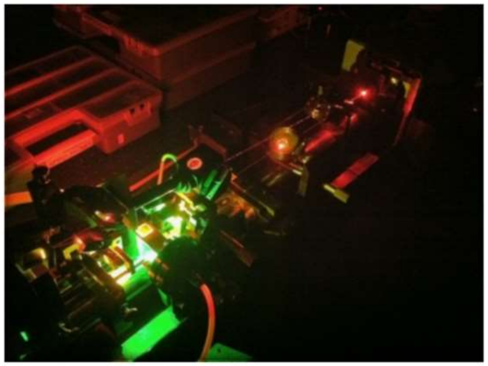
$Si(CH_3)_3OH$

trimethylsilanol (TMS)



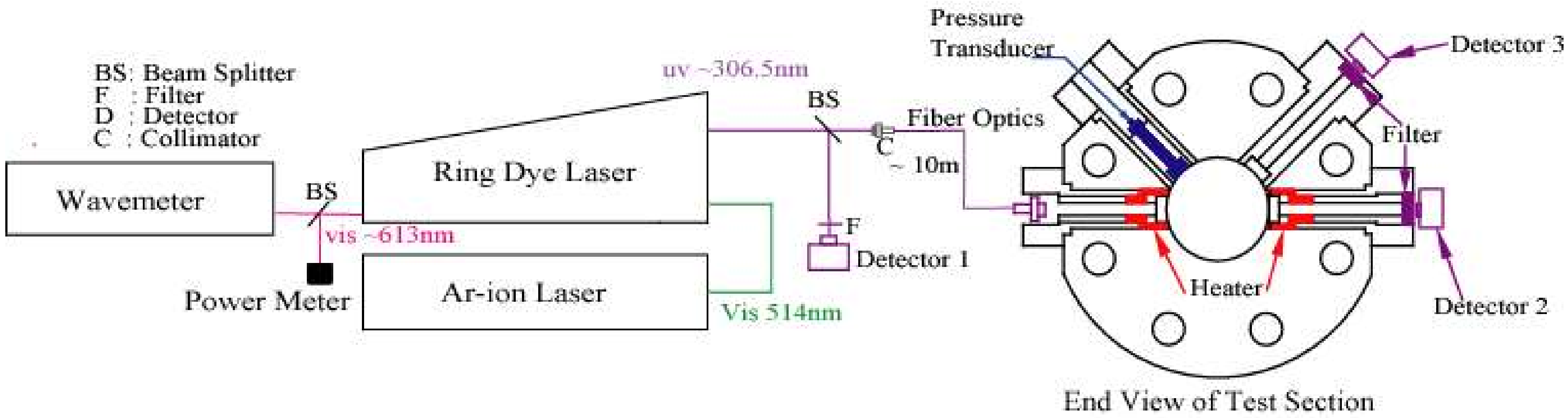
$(CH_3)_3SiOSi(CH_3)_3$

hexamethyldisiloxane (HMDSO)



Thank you!

Questions/Comments?



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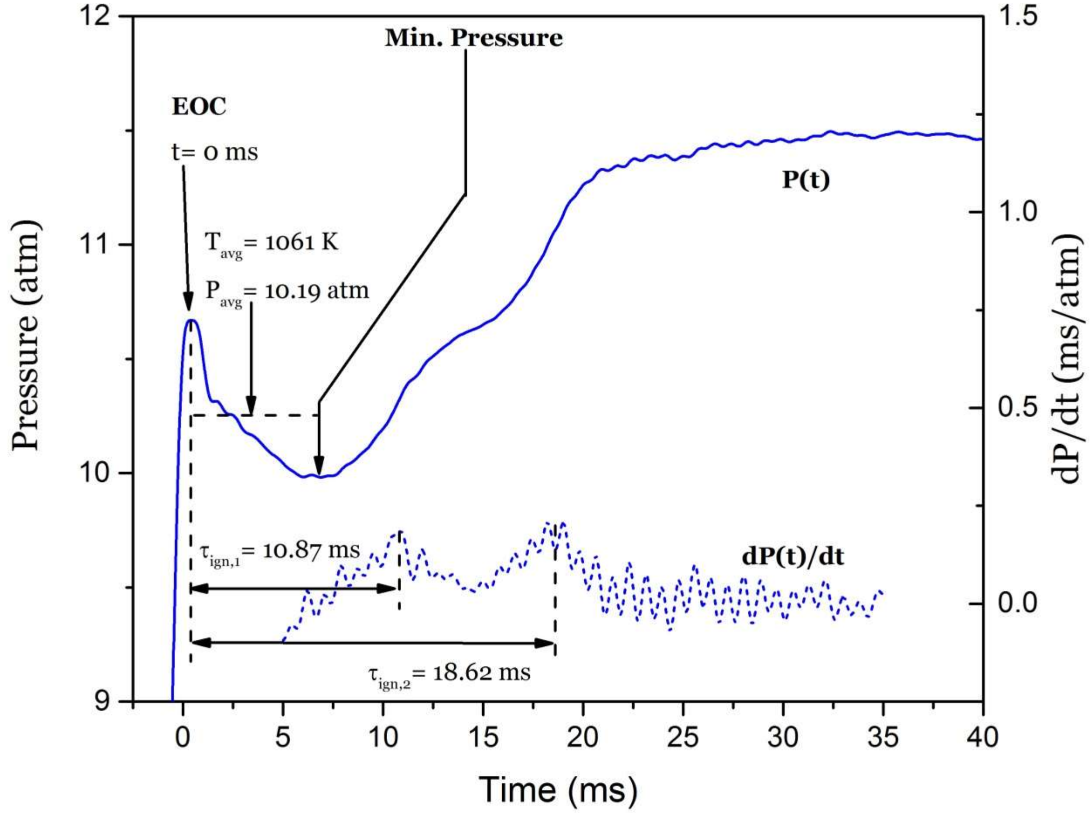
Methods: typical results and analysis

Typical Pressure Trace



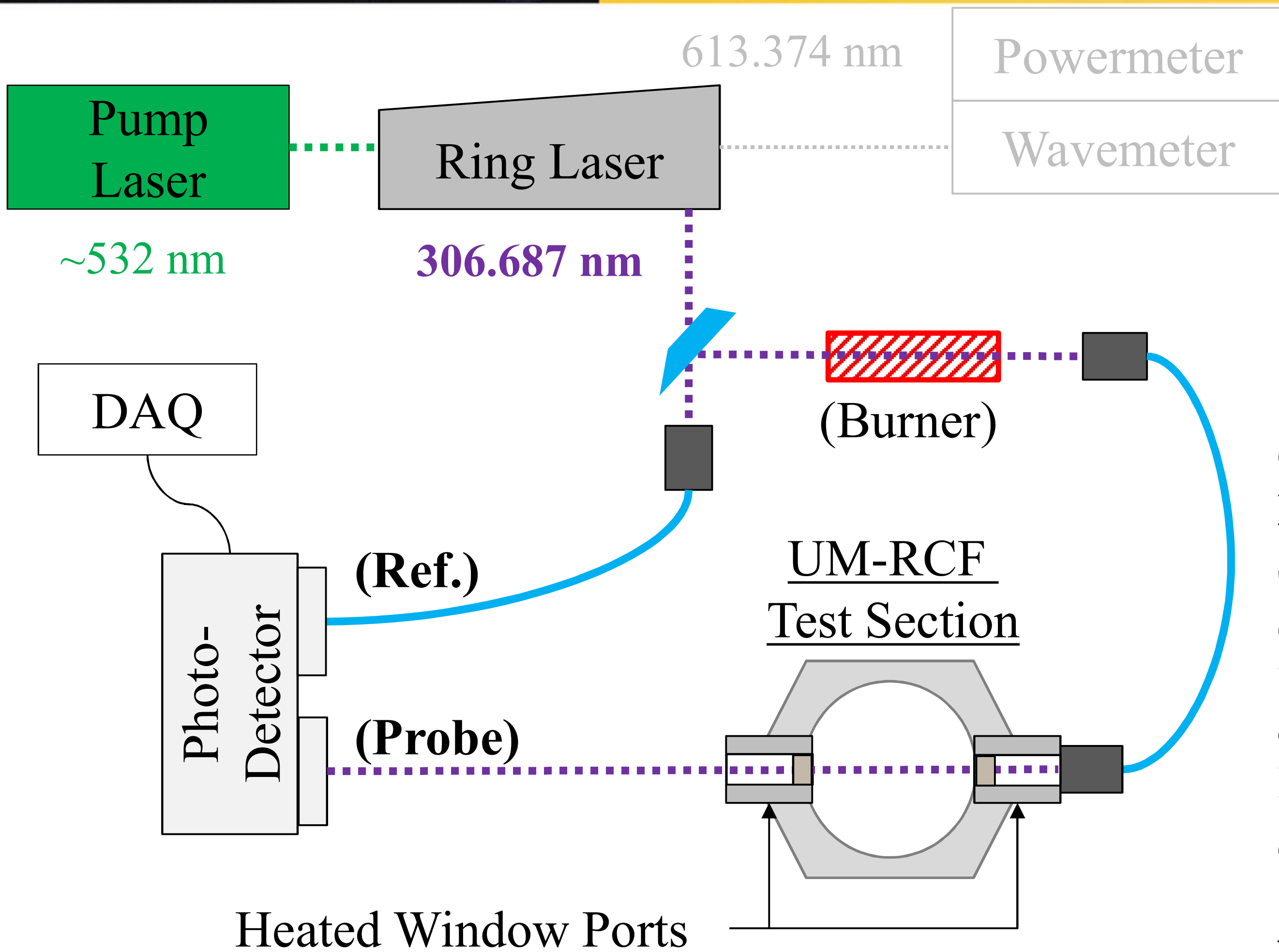
Analysis

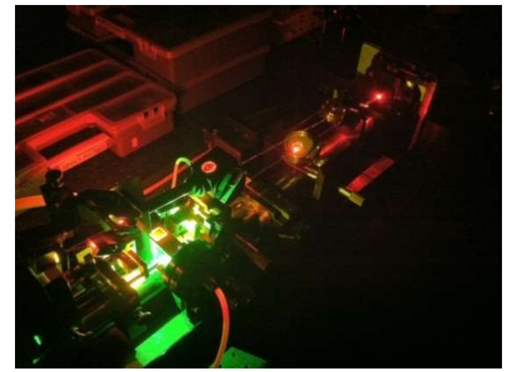
Average thermodynamic state assigned to capture heat loss at EOC

τ_{ign} = time @ max $\left|\frac{dP}{dt}\right|$ for second stage

τ_{ign1} = time @ max $\left|\frac{dP}{dt}\right|$ for first stage

New OH Laser Absorption System





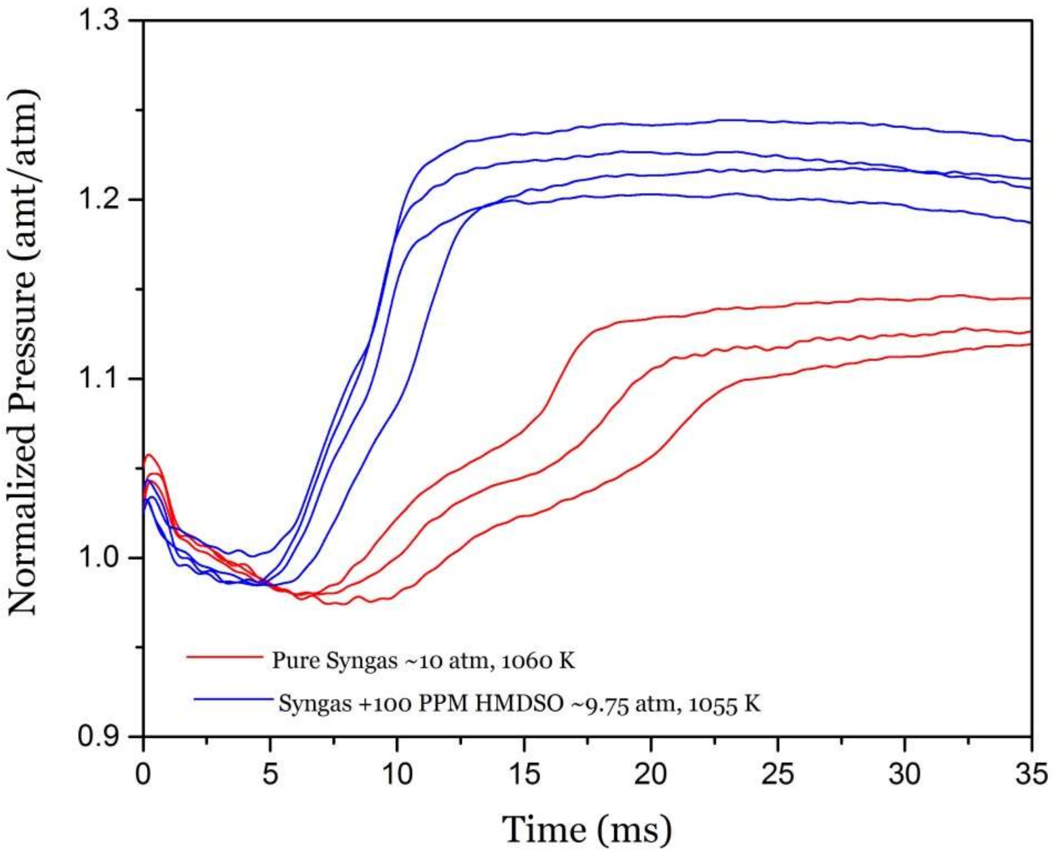
Goal
Measure $\chi_{OH}(t)$ during syngas auto-ignition.

Conditions
P ~ 5 atm, T ~ 1000-1090 K
φ = 0.1, ~Air Dil., N_2 (Ar)
Fuel: 30% H_2, 70% CO

Computations
Li 2007 mech.
NUIG 2013 mech. [19]

- Low precision targets dominate (τ_{ign}, s_L^o) available kinetic data
- Important O, OH, H radical data very limited for H_2 (high-T, low-P, ultra dilute) [29], unstudied for syngas

Results: effects of HMDSO on syngas ignition

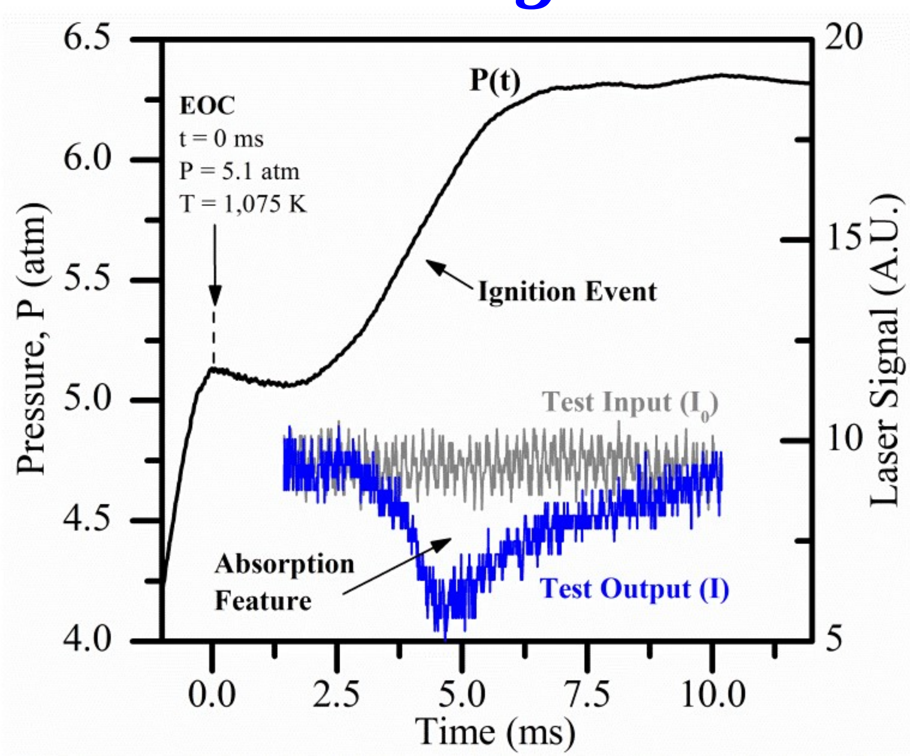


- Pressures 9.5-10.2 atm, Temperatures 1050-1062 K
- (1) Pure syngas
  (2) Syngas + 100 ppm HMDSO
- Pressure trace normalized by effective pressure

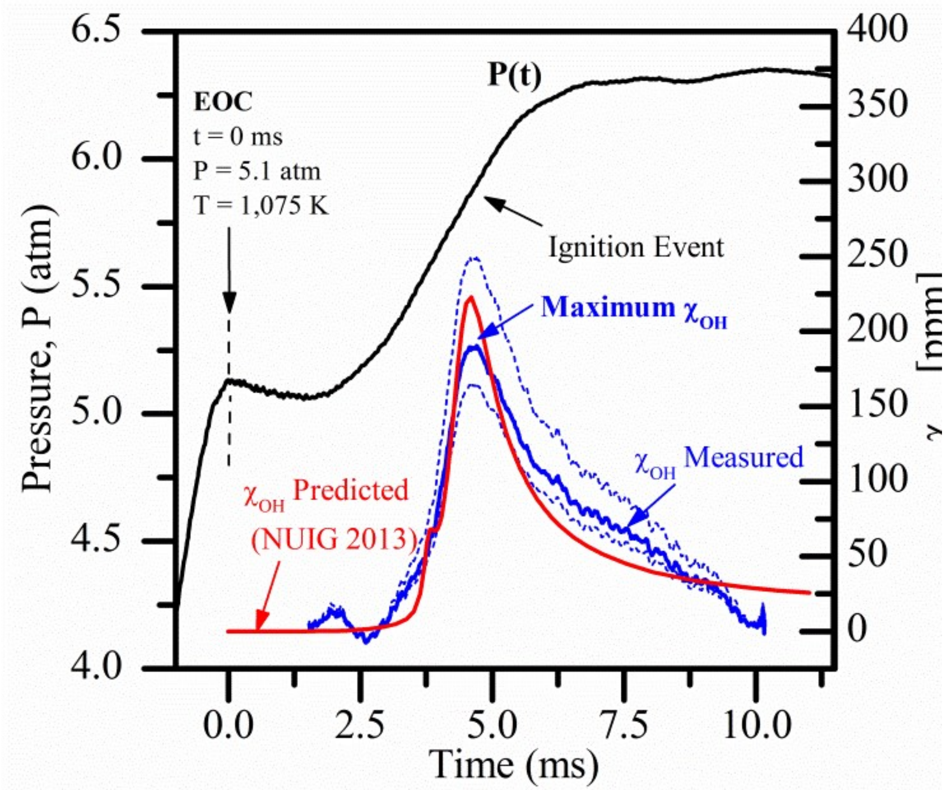
- Ignition delay noticeably decreased with addition of 100 ppm HMDSO
- Magnitude of pressure increase is greater with HMDSO
- Two stage heat release apparent with and without HMDSO

Typical χ_{OH} time history

Raw Signals

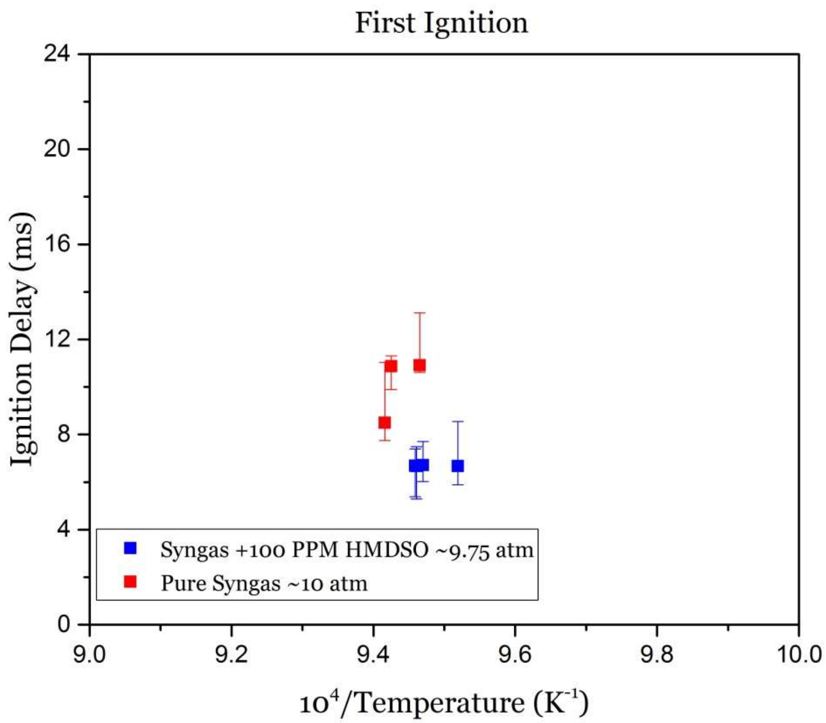


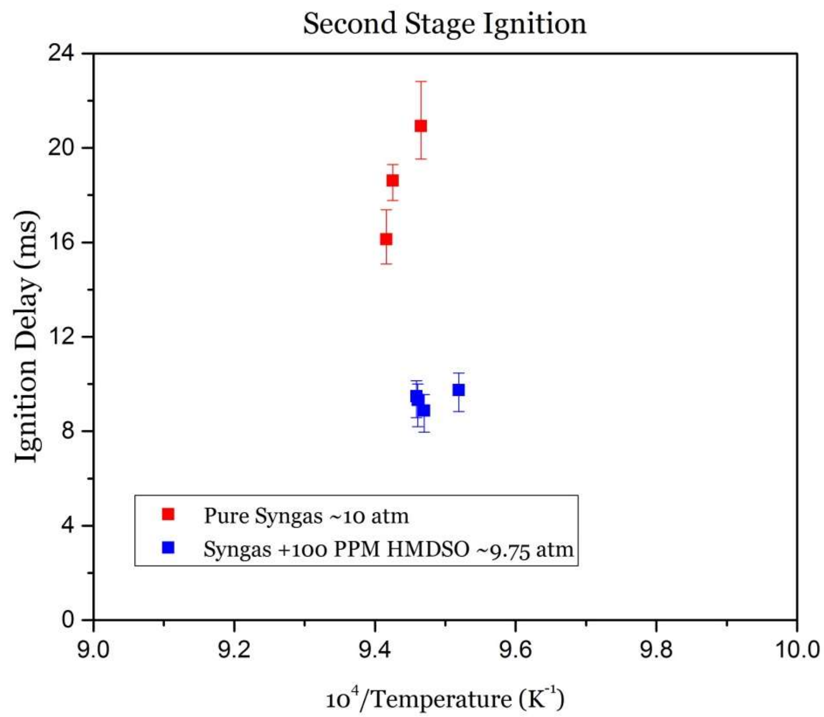
$\chi_{OH}(t)$



- Clear absorption feature
- Excellent agreement between measured and predicted $\chi_{OH}(t)$
- Interrogation of multiple features possible (magnitudes, slopes), to improve chemical kinetics

Results: effects of HMDSO on syngas ignition

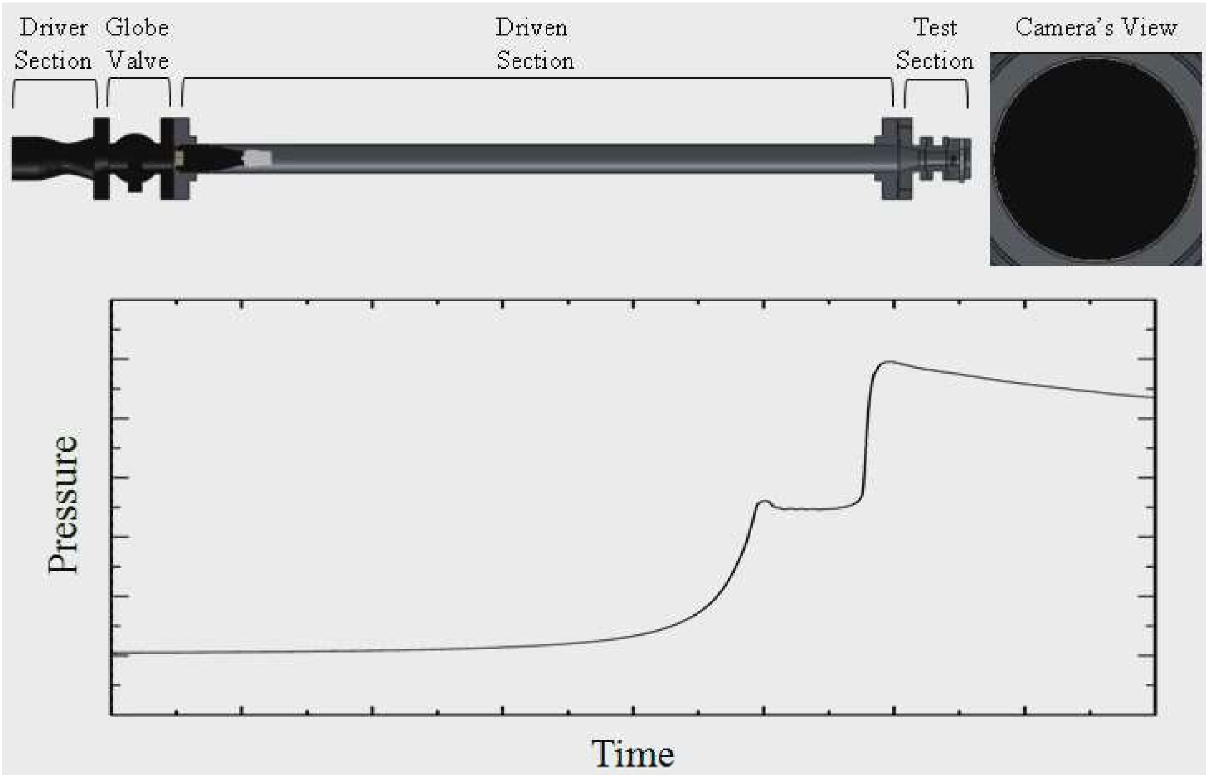


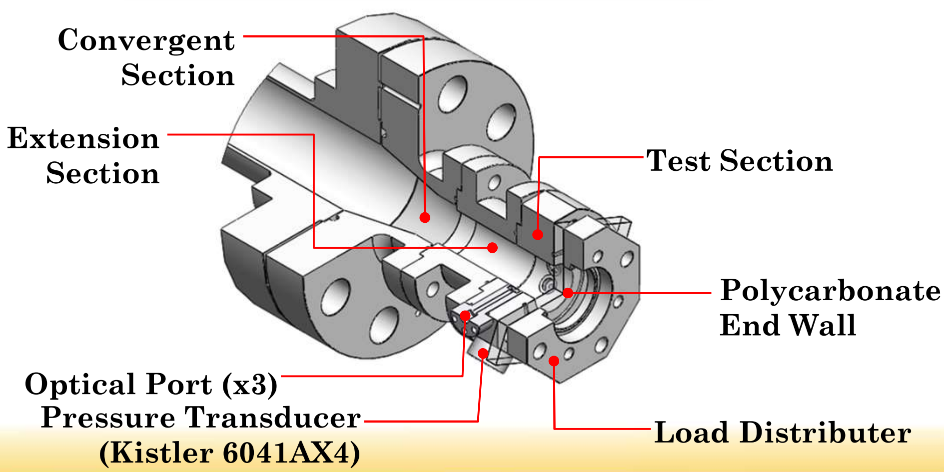


- Delay times for both first and second ignition decreased with 100 ppm HMDSO
- Second ignition delay time decreased by ~ factor of 2 with 100 ppm HMDSO

combustion LABORATORY

UM RCF: experimental setup for ignition studies





EOC pressures from 0.5 to 30 atm by varying:

- Compression ratio
- Nosecone design
- Fill pressure

Isentropic compression in the core

- $T_{axis} \approx T_S \pm 5\% T_S$
- 65% of V at $\pm$ 10%T_{axis}

Test section dimensional characteristics:

- V≈ 200 cm3
- V : $A_S \approx$ 0.8-1.1

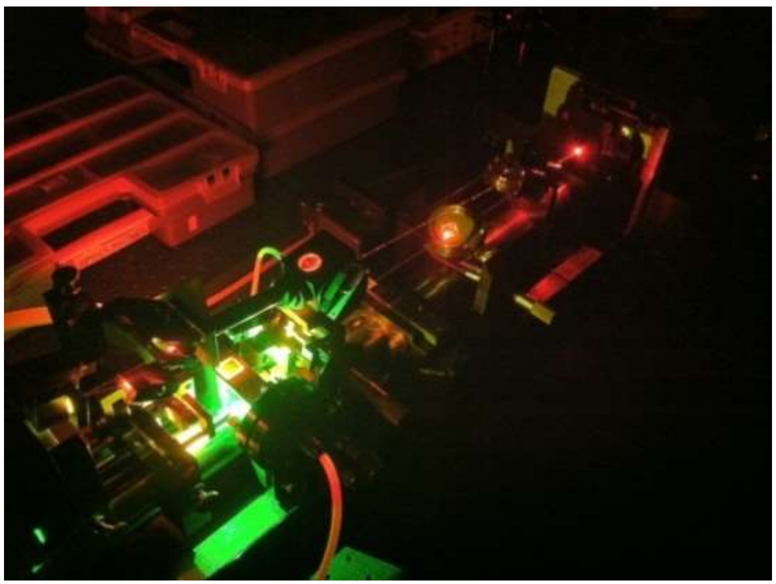
Ignition test times from 1 to 60 ms

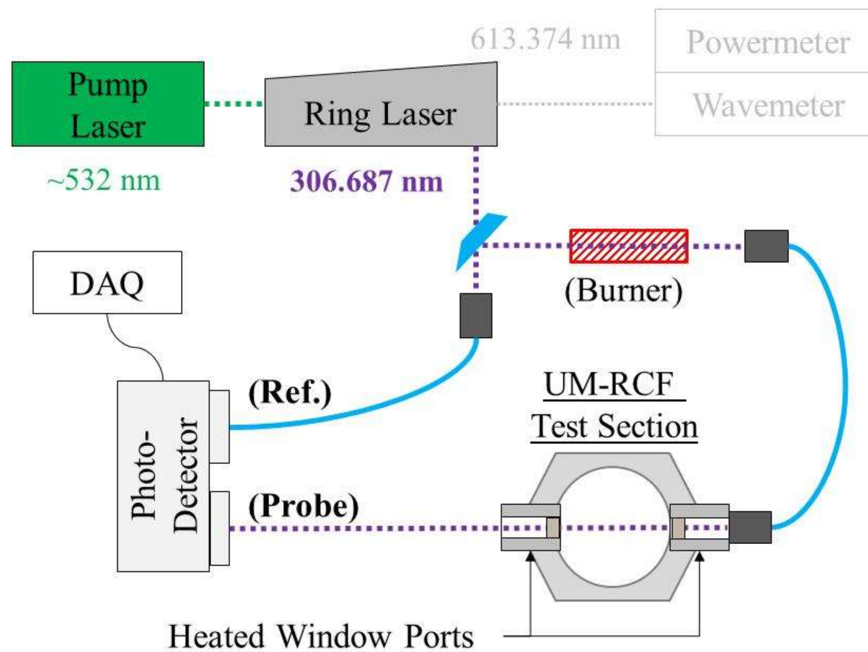
$$P_{\text{eff}} = \frac{1}{(t_{P_{\min}} - t_{P_{\max}})} \int_{t_{P_{\max}}}^{t_{P_{\min}}} P \, dt$$

$$\int_{T_0}^{T_{\text{eff}}} \frac{\gamma}{\gamma - 1} \, d \ln T = \ln\left(\frac{P_{\text{eff}}}{P_0}\right)$$

Current work on ignition impurities

- Expanding the ignition data set on HMDSO
- Interpreting of the effects of TMS and the effects of HMDSO, based on chemical structure and H_2/CO elementary chemical kinetics
- OH measurements during ignition of syngas with and without TMS and HMDSO
  - Laser system restarted after building renovations
  - Thick-etalon assembly replaced





Current work : OH measurements

Goal
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Conditions
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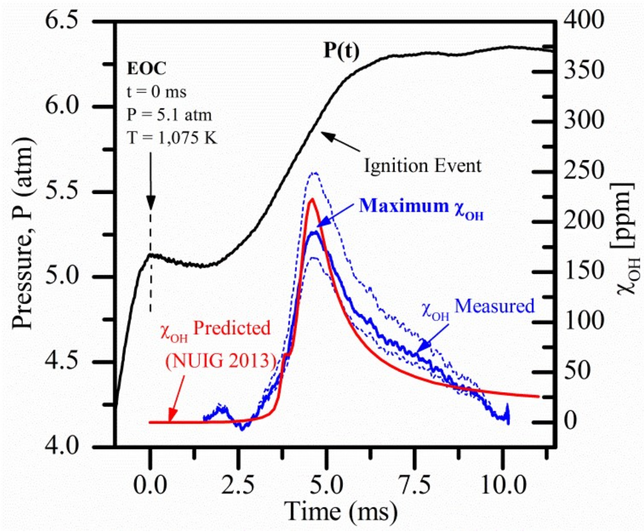
Fuel: 30% H_2, 70% CO, with and without TMS and HMDSO impurities

- Low precision targets dominate (τ_{ign}, s_L^o) available kinetic data
- Important O, OH, H radical data very limited for H_2 (high-T, low-P, ultra dilute) [29], unstudied for syngas

  - Previous UM RCF work showed visible OH absorption feature
  - Excellent agreement between measured and predicted $\chi_{OH}(t)$
  - Interrogation of multiple features possible (magnitudes, slopes), to improve chemical kinetics



Turbulence Extension of Sa

Sankaran (Zeldovich) Number (RANS/LES "Turbulence" Version)

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} = \beta S_L \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) |\nabla T| \approx \beta S_L \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \widetilde{|\nabla T|}$$

where

$$\widetilde{|\nabla T|} = \frac{T'}{\lambda_T} \approx \frac{T'}{\lambda} = \frac{T'}{\ell \, \mathrm{Re}_\ell^{-1/2}}$$

hence

$$\mathrm{Sa} = \beta S_L \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \frac{T'}{\ell} \mathrm{Re}_\ell^{1/2}$$

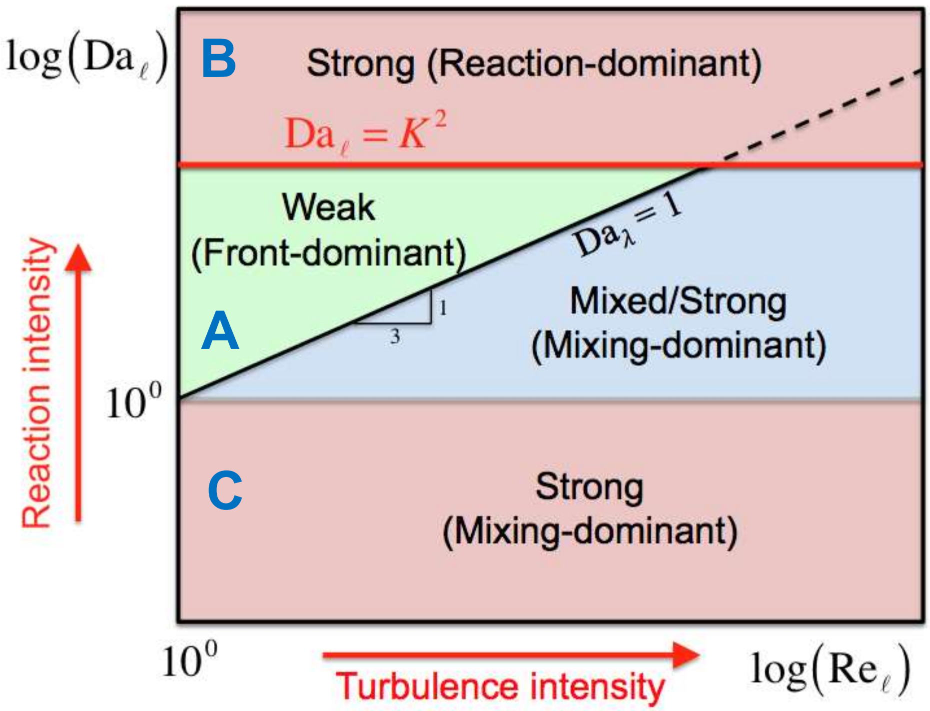
$$= \beta \left(\frac{S_L}{\delta_f} \right) \left(\frac{\delta_f}{\ell} \right) T' \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \mathrm{Re}_\ell^{1/2}$$

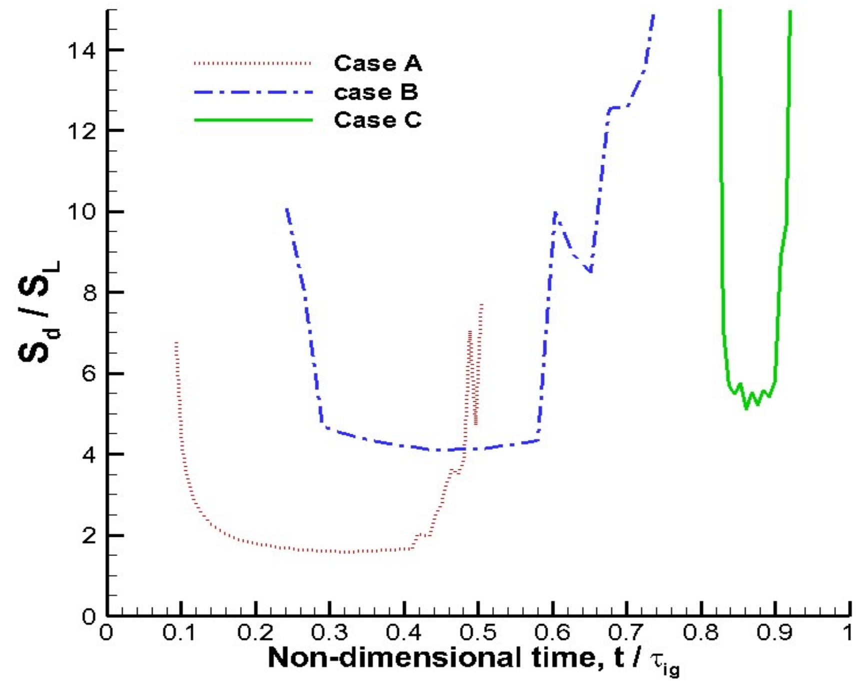
$$\begin{cases} \mathrm{Sa} > 1 & \text{Weak} \\ \mathrm{Sa} < 1 & \text{Strong} \end{cases}$$

$$\delta_f = \frac{\alpha}{S_L}$$ (nominal) flame thickness

$$= \beta \left(\frac{1}{\tau_f} \right) \mathrm{Re}_\ell^{-1/2} \mathrm{Da}_\ell^{-1/2} \left(\frac{\tau_{ig}}{\tau_f} \right)^{-1/2} T' \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \mathrm{Re}_\ell^{1/2} = \beta \left(\frac{T'}{\tau_f} \right) \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right) \left[\mathrm{Da}_\ell \left(\frac{\tau_{ig}}{\tau_f} \right) \right]^{-1/2}$$

Front Propagation Speeds

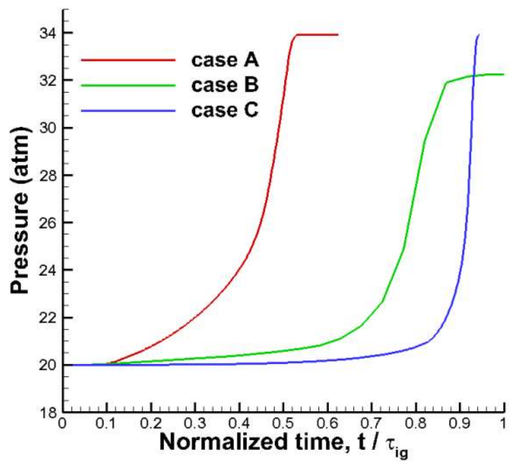


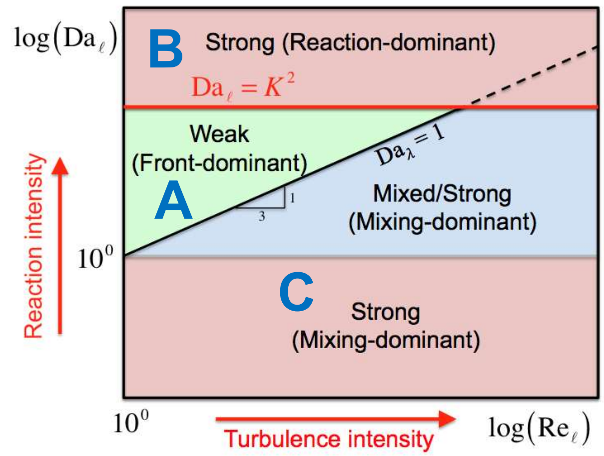


For case A, the minimum front speed is close to S_L, indicating deflagrative front propagation.

For cases B and C, the minimum front speed is much higher (by over a factor of 4) than S_L, suggesting that spontaneous propagation is the dominant combustion mode.

Regime diagram validation
2D DNS: Evolution of temperature field

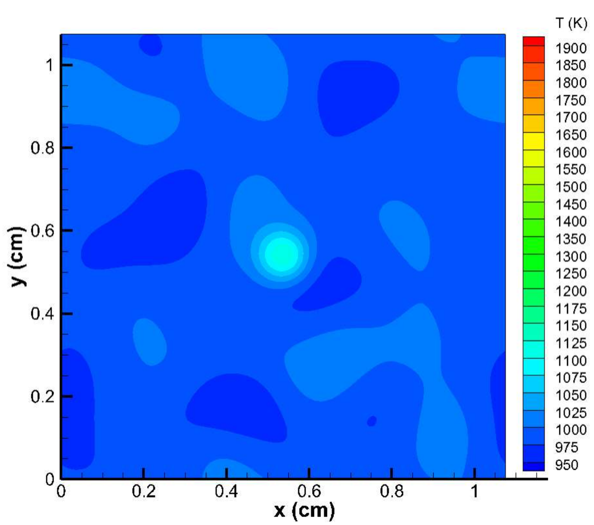


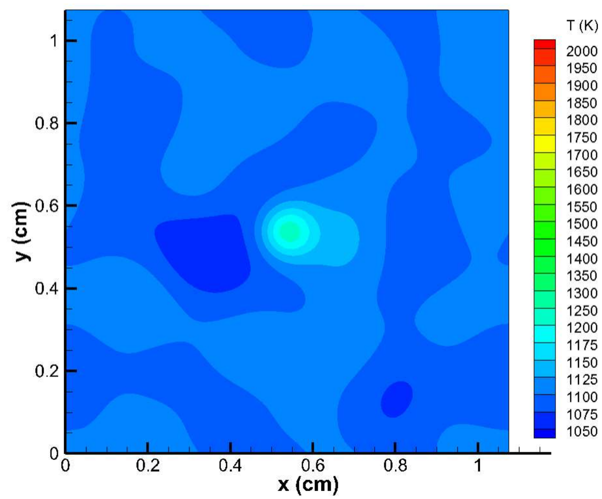


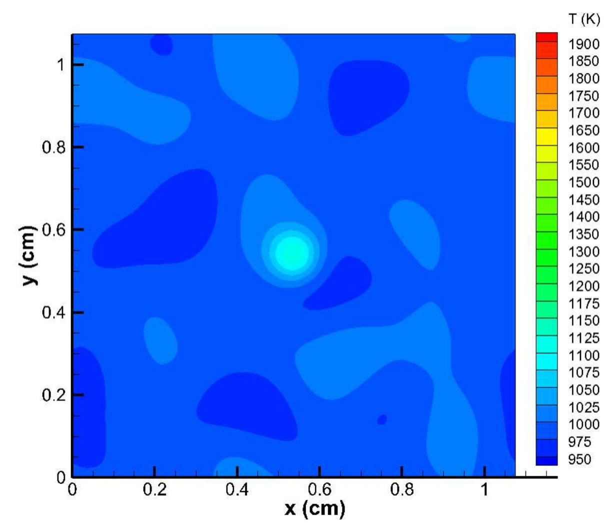
A. Weak Ignition

B. Strong Ignition (Reaction-dominant)

C. Strong Ignition (Mixing-dominant)

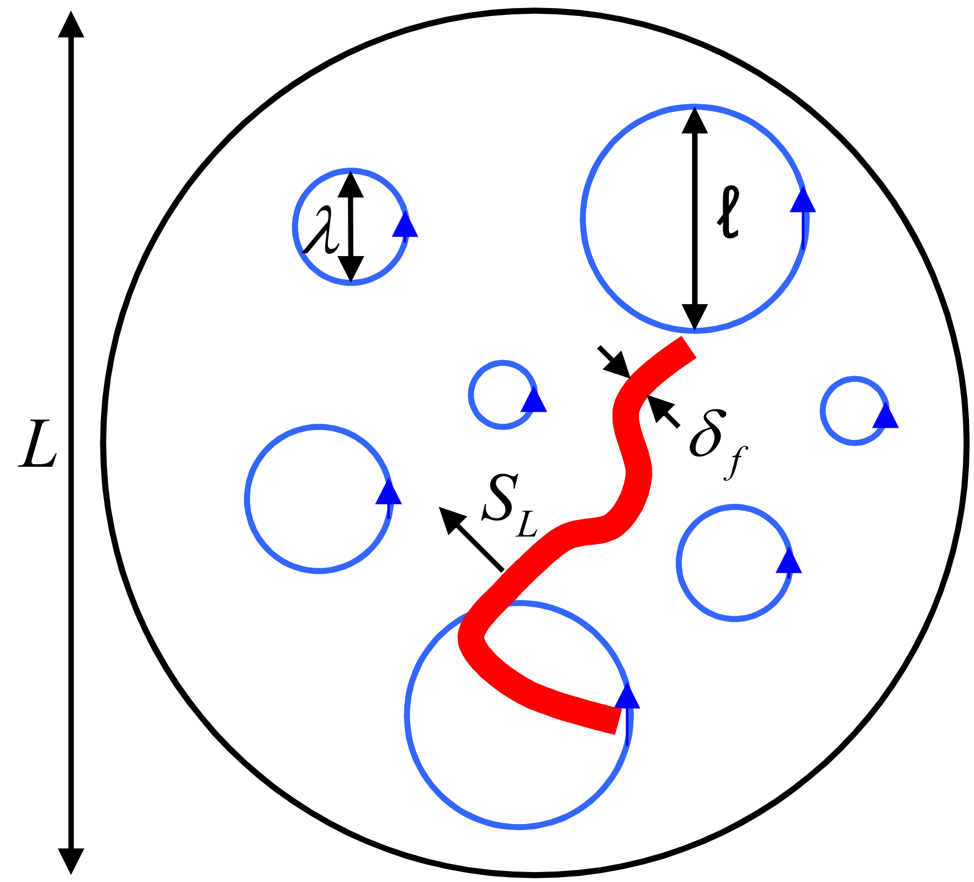






Schematic of Scales

Im, Pal, Woodridge, Mansfield, *Combustion, Science and Technology* (2015)



L : chamber length (not considered)

ℓ : integral eddy scale

λ : Taylor microscale $\left(=\lambda_T\right)$

δ_f : Deflagration flame thickness

S_L : Laminar flame speed

Homogeneous turbulence:

$$\frac{\ell}{\lambda} = \mathrm{Re}_{\ell}^{1/2} = \left(\frac{u'\ell}{\nu}\right)^{1/2} ; \quad \frac{u'}{u'_{\lambda}} = \left(\frac{\ell}{\lambda}\right)^{1/3}$$