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# Regimes of Autoignition in Nearly Homogeneous Syngas Mixtures

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# Discrepancies in Ignition Delay Times

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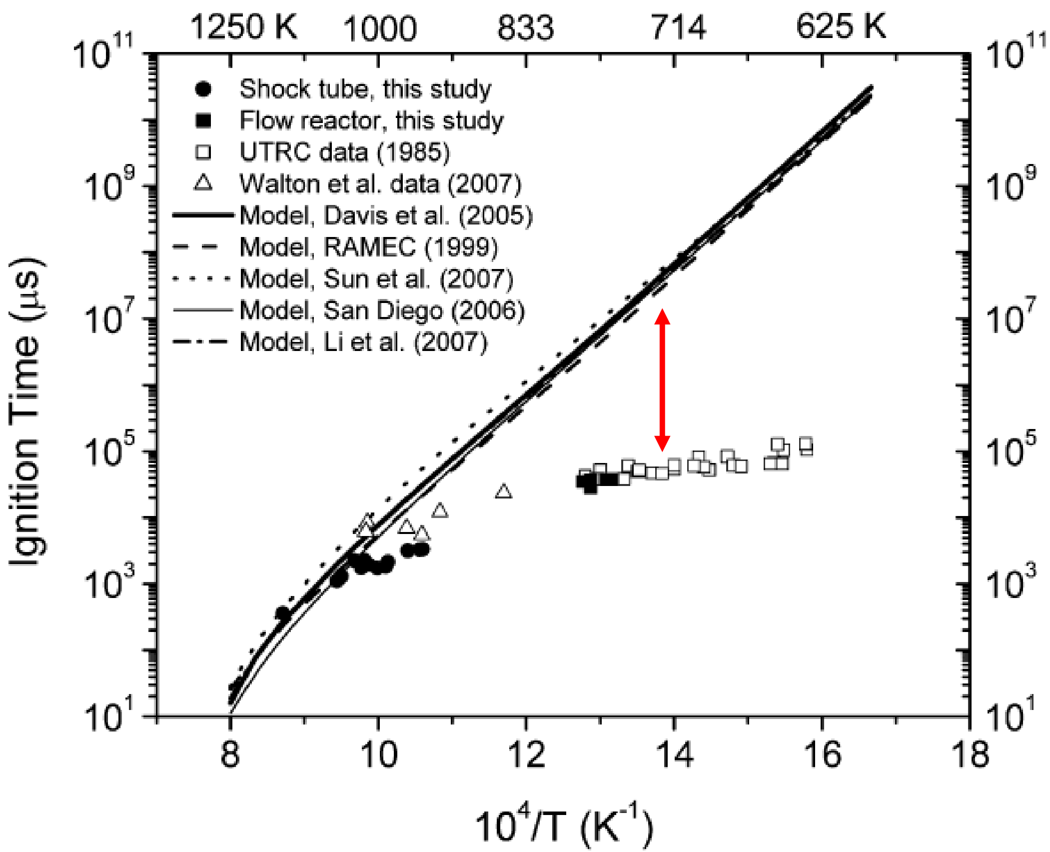
Petersen et al., 2007



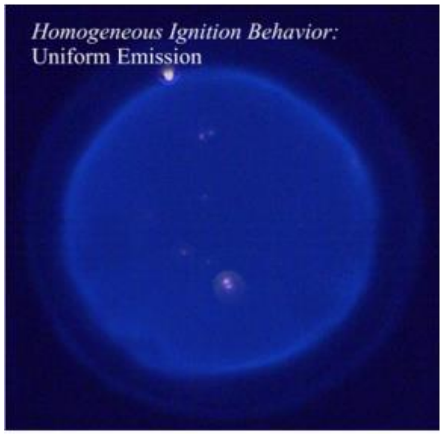

Discrepancy in ignition delay between the experiments and numerical modeling has not been fully understood.

Possible explanations:

- Uncertainties in Rate Coefficients
- Incomplete Reaction Mechanisms
- Surface-Catalytic Mechanisms
- Ignition Regimes
- Wall Heat Transfer
- Turbulence

# “Weak” versus “Strong” Ignition

Mansfield and Wooldridge, C&F 2014

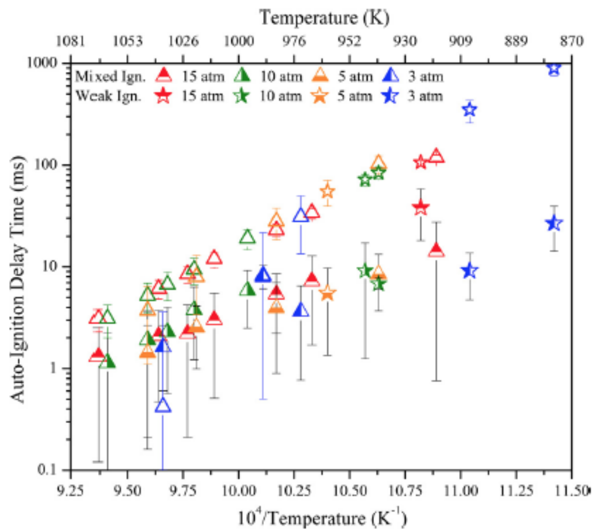


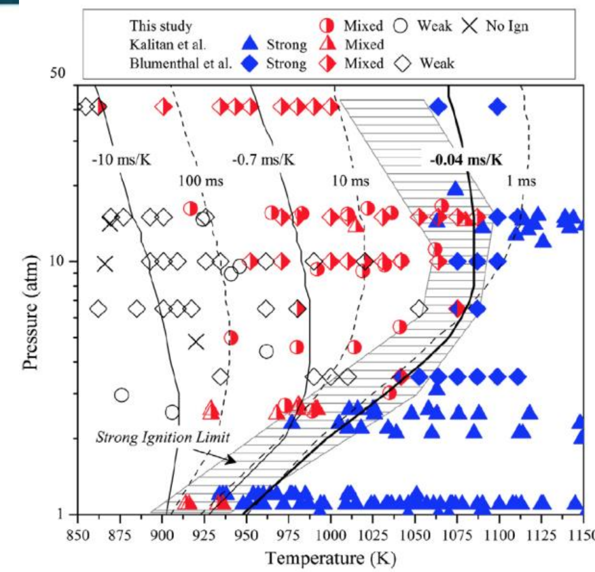

P = 3.3 atm, T = 1043 K, φ = 0.1

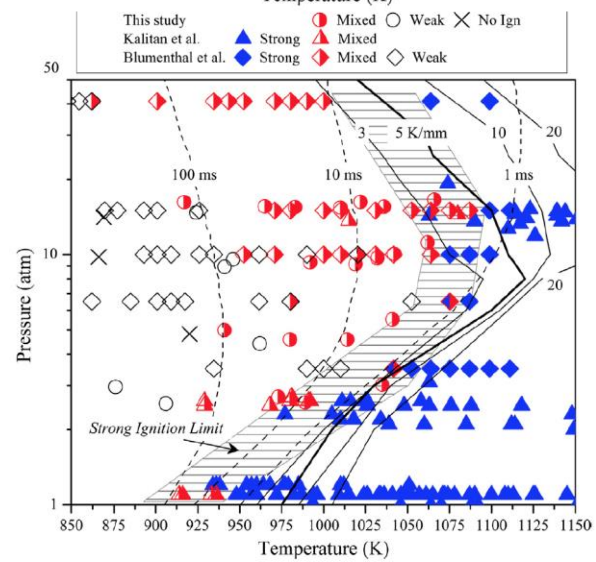

P = 9.2 atm, T = 1019 K, φ = 0.5

Weak ignition results in noticeable differences in the ignition delay times.

Ignition regimes mapped for either $dt_{ig} / dT$ (property) or $dT / dx$ (condition).



# Turbulence-Chemistry Interaction

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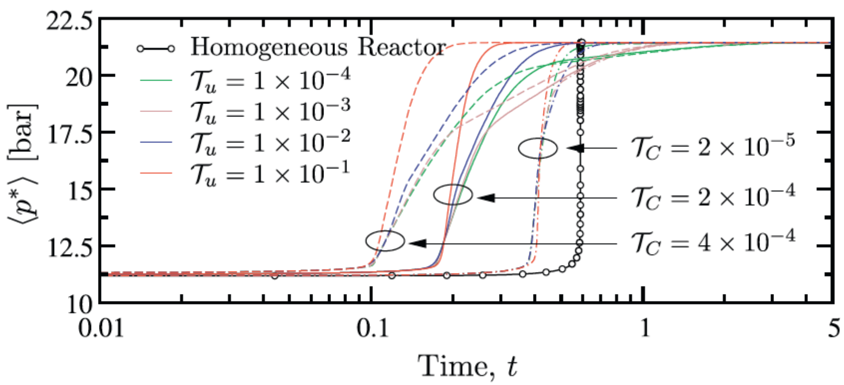
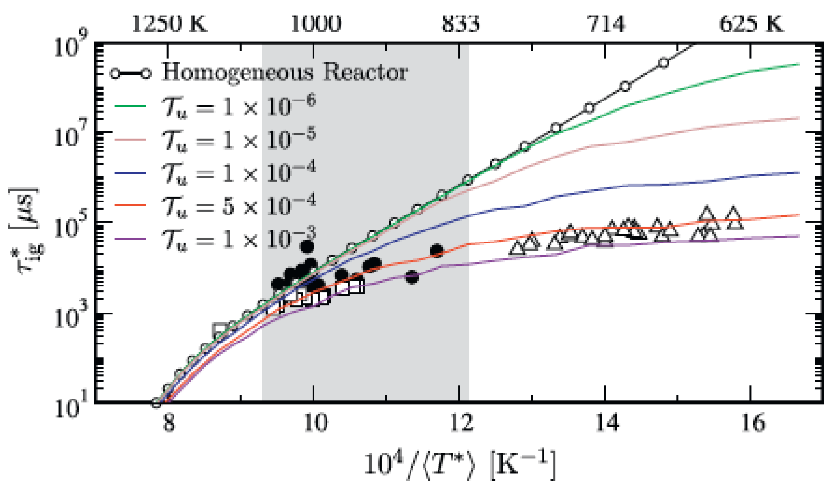
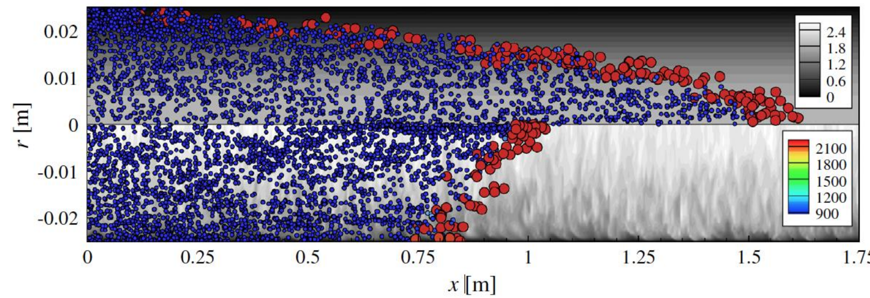
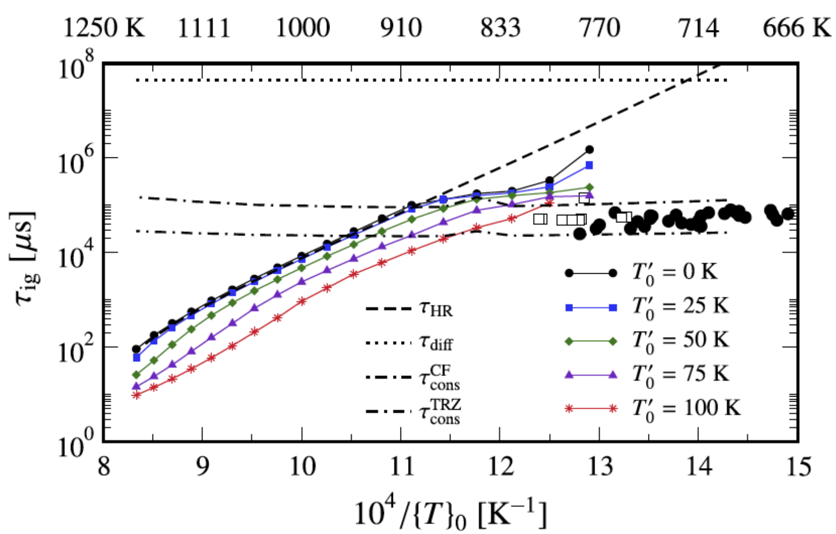
## Ihme, C&F 2012
## 0D model prediction




## Wu & Ihme, C&F 2014
## Lagrangian model prediction



# Shock-induced Ignition

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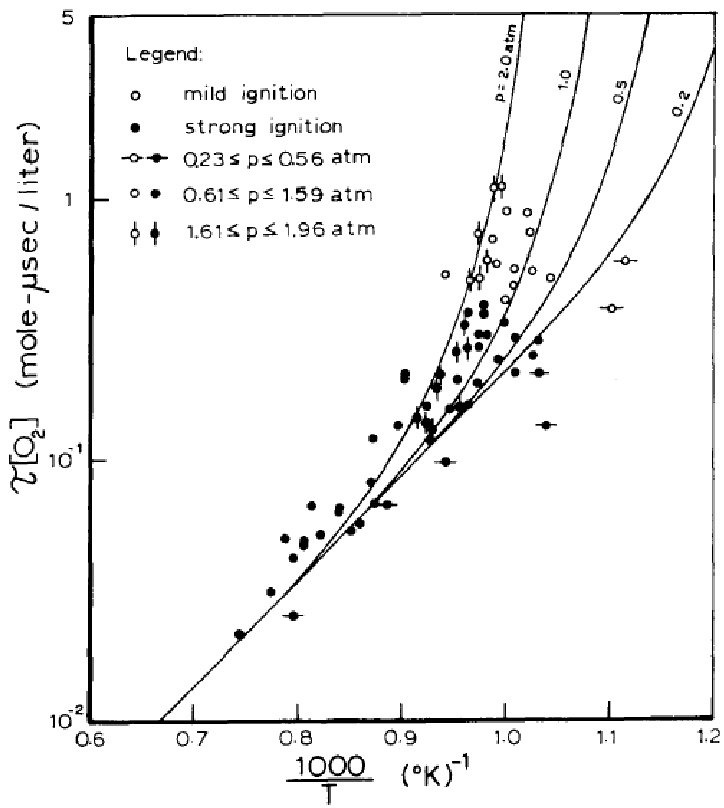
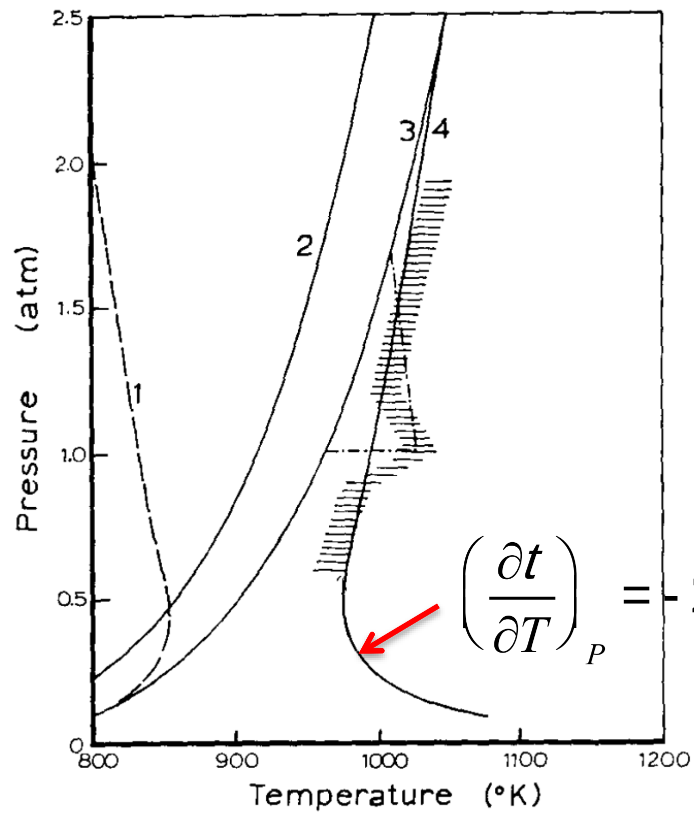
## Meyer and Oppenheim, 13$^{th}$ Symposium (1970)




$$\left(\frac{\partial t}{\partial T}\right)_P = -2\ \mu\text{sec/K}$$

*"However, the nonuniformities are of lesser importance at higher temperatures where the induction time is, on one hand, less sensitive to temperature variation and, on the other, it is too short with respect to the characteristic time for transport phenomena to allow the latter to influence the development of the process."*

# Weak Ignition in Shock Tubes

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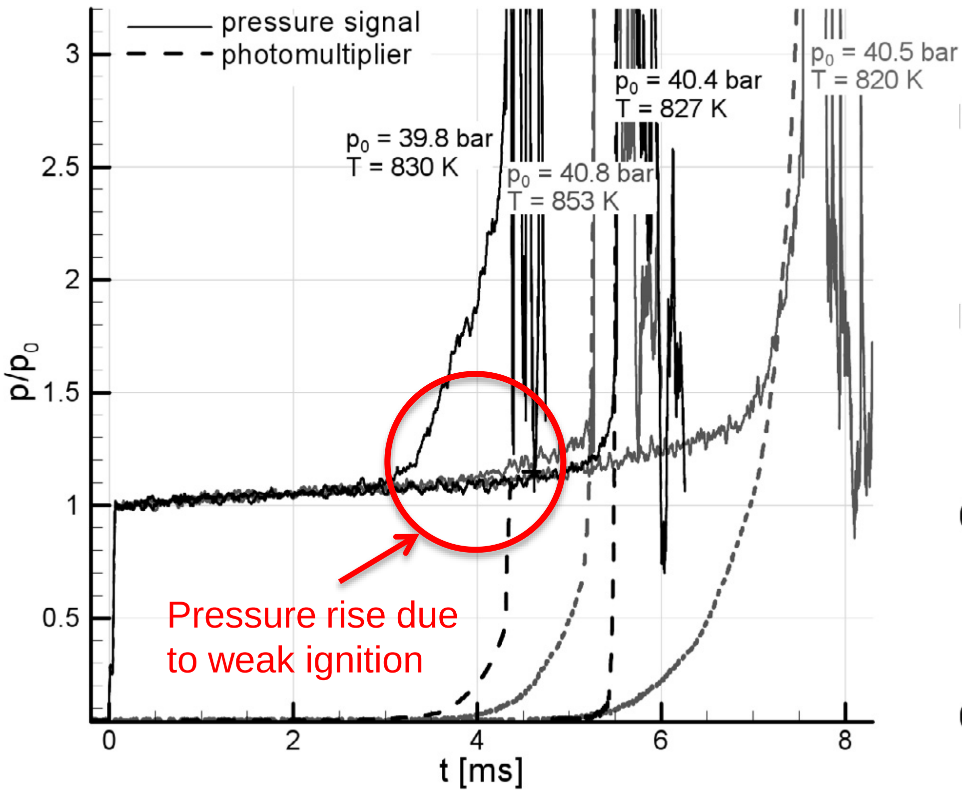
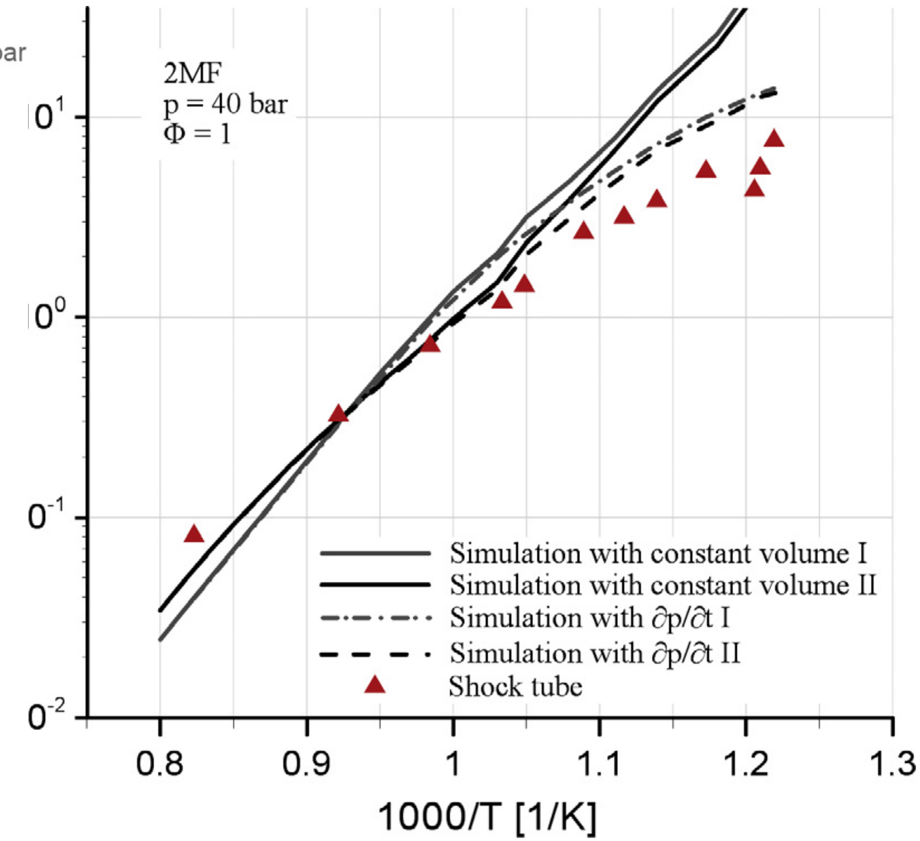
Uygun, Ishihara, Olivier, C&F 2014



# KAUST Shock Tubes

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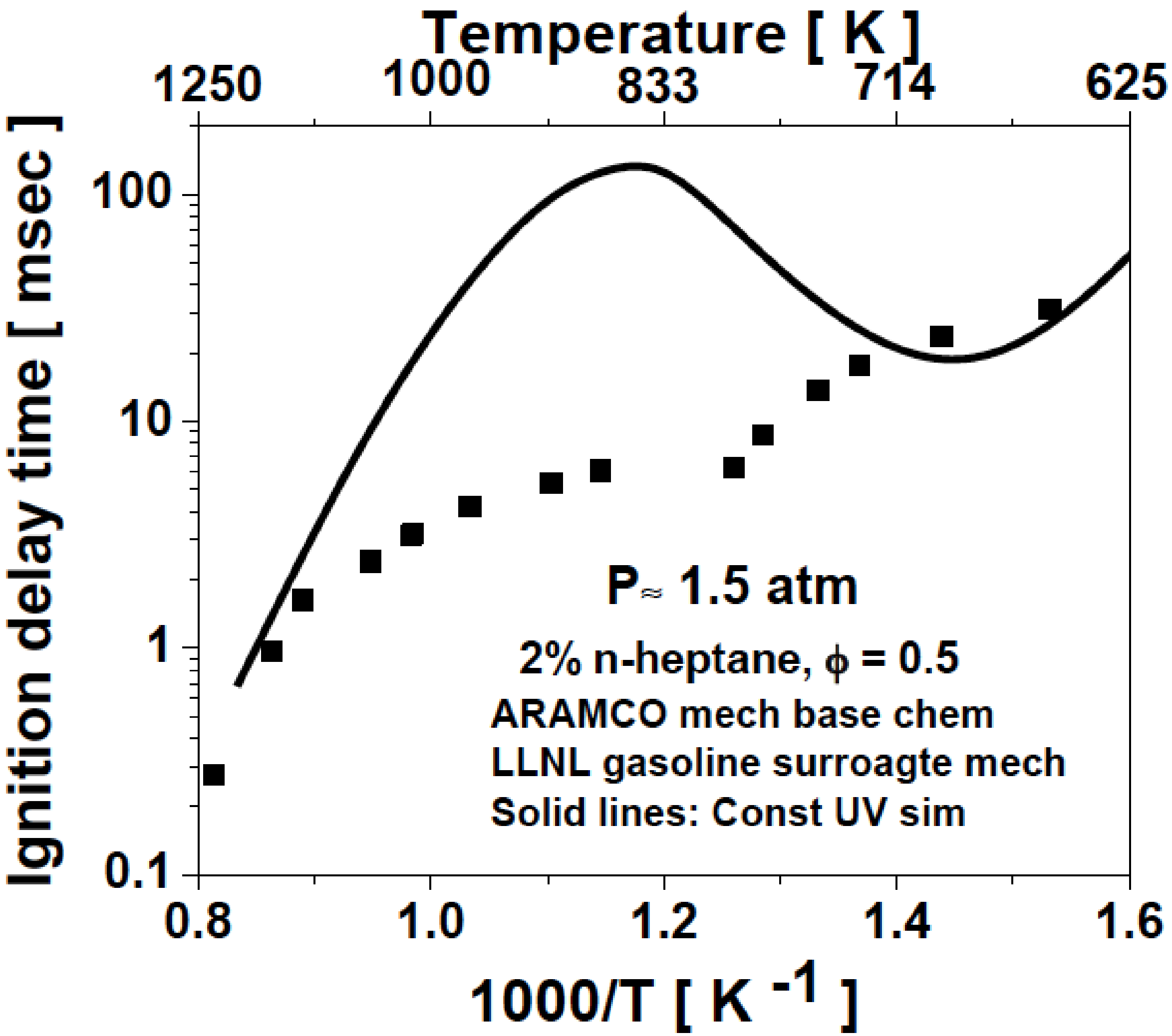
Javed & Farooq, KAUST Low Pressure Shock Tube Facility



# Key Questions

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The Sankaran (Zeldovich) Criterion:

$$\mathrm{Sa} = b\frac{S_L}{S_{sp}} = bS_L\left(\frac{dt_{\mathrm{ig}}}{dT}\right)\left(\frac{dT}{dx}\right) \qquad b \gg 0.5$$

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

- Does the criterion serve as a unified metric for separating weak vs. strong ignition?
- How do we extend the criterion in turbulent conditions?

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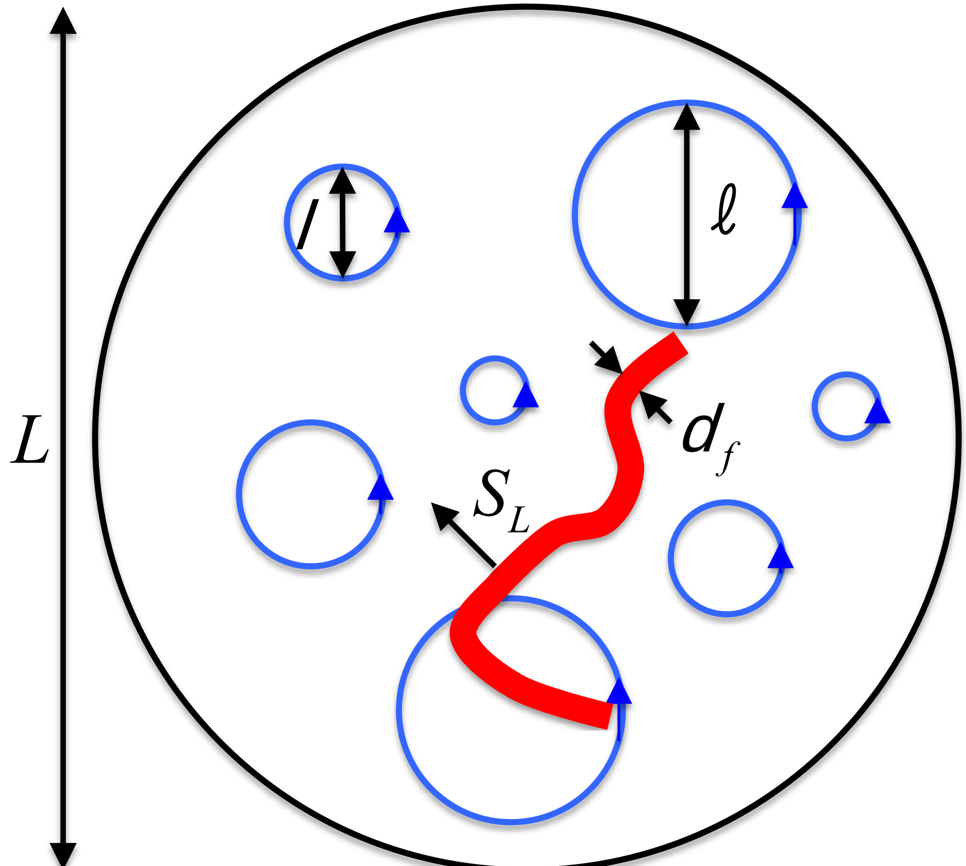
# Schematic of Scales




$L$ : chamber length (not considered)

$\ell$ : integral eddy scale

$l$ : Taylor microscale $\left(= l_T\right)$

$d_f$ : Deflagration flame thickness

$S_L$ : Laminar flame speed

Homogeneous turbulence:

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

# Assumptions & Hypotheses



- Weak ignition is triggered by small-scale fluctuations (e.g. local hot spots), and effect of large-scale bulk temperature gradient is not considered (the results can be extended).

- Scales of temperature and velocity fluctuations are comparable and correlated.

- Pr = 1: Dissipation of temperature fluctuations is mainly due to turbulent flows, and thus the time and length scales for turbulent and scalar energy are the same (Batchelor scale = Kolmogorov scale)

# Relevant Nondimensional Numbers

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## Measure of turbulence intensity

Turbulent Reynolds number: $$\mathrm{Re}_\ell = \frac{u'\ell}{\nu}$$

## Measure of reaction intensity

Ignition Damköhler numbers:

$$\mathrm{Da}_\ell = \frac{\tau_\ell}{\tau_{ig}}$$ Integral Da – based on integral scale eddies

$$\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{\mathrm{ig}}}$$ Mixing Da – based on mixing (Taylor) scale eddies

where the mixing time and scale is determined by

$$\tau_{\lambda_T} = \frac{T'^2}{2\alpha\overline{|\nabla T|^2}}, \lambda_T^2 = \frac{T'^2}{\overline{|\nabla T|^2}}$$

$T'$: RMS temperature fluctuation

# Da-Re Relations

Based on assumption that temperature mixing is similar to turbulence mixing (i.e. Kolmogorov scale = Batchelor scale),

$$t_{l_T} = t_l; \quad l_T = l$$

It follows that

$$\mathrm{Da}_l = \frac{t_{l_T}}{t_{\mathrm{ig}}} = \frac{t_l}{t_{\mathrm{ig}}} = \frac{t_\ell}{t_{\mathrm{ig}}} \frac{t_l}{t_\ell} = \mathrm{Da}_\ell \, \mathrm{Re}_\ell^{-1/3}$$

$$\left( \frac{t_l}{t_\ell} = \frac{l / u'_l}{\ell / u'} = \frac{l}{\ell} \frac{u'_l}{u'} = \left( \frac{l}{\ell} \right)^{2/3} = \mathrm{Re}_\ell^{-1/3} \right)$$

# Weak vs. Strong Ignition Criterion

Sankaran (Zeldovich) Number (DNS "Fully Resolved" Version)

$$\mathrm{Sa} = b\frac{S_L}{S_{sp}} = bS_L\left[\frac{dt_{\mathrm{ig}}}{dT}\frac{dT}{dx}\right] = bS_L\left[\frac{dt_{\mathrm{ig}}}{dT}\left|\nabla T\right|\right] \qquad \left(b \text{ » } 0.5\right)$$

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

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

# Turbulence Extension of Sa

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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

$$\mathrm{Sa} = bS_L \left(\frac{dt_{\mathrm{ig}}}{dT}\right) \frac{T'}{\ell} \mathrm{Re}_\ell^{1/2}$$

$$= b\left(\frac{S_L}{d_f}\right)\left(\frac{d_f}{\ell}\right) T' \left(\frac{dt_{\mathrm{ig}}}{dT}\right) \mathrm{Re}_\ell^{1/2}$$

$$= b\left(\frac{1}{t_f}\right) \mathrm{Re}_\ell^{-1/2} \mathrm{Da}_\ell^{-1/2} T' \left(\frac{dt_{\mathrm{ig}}}{dT}\right) \mathrm{Re}_\ell^{1/2} = b\left(\frac{T'}{t_f}\right)\left(\frac{dt_{\mathrm{ig}}}{dT}\right) \mathrm{Da}_\ell^{-1/2}$$

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

$$d_f = \frac{a}{S_L}$$ (nominal) flame thickness

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# Regime Criteria

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Turbulent Sankaran Number:

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

where $K = b\left(\dfrac{T'}{t_f}\right)\left(\dfrac{dt_{\mathrm{ig}}}{dT}\right)$ Nondimensional ignition sensitivity

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

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

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

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

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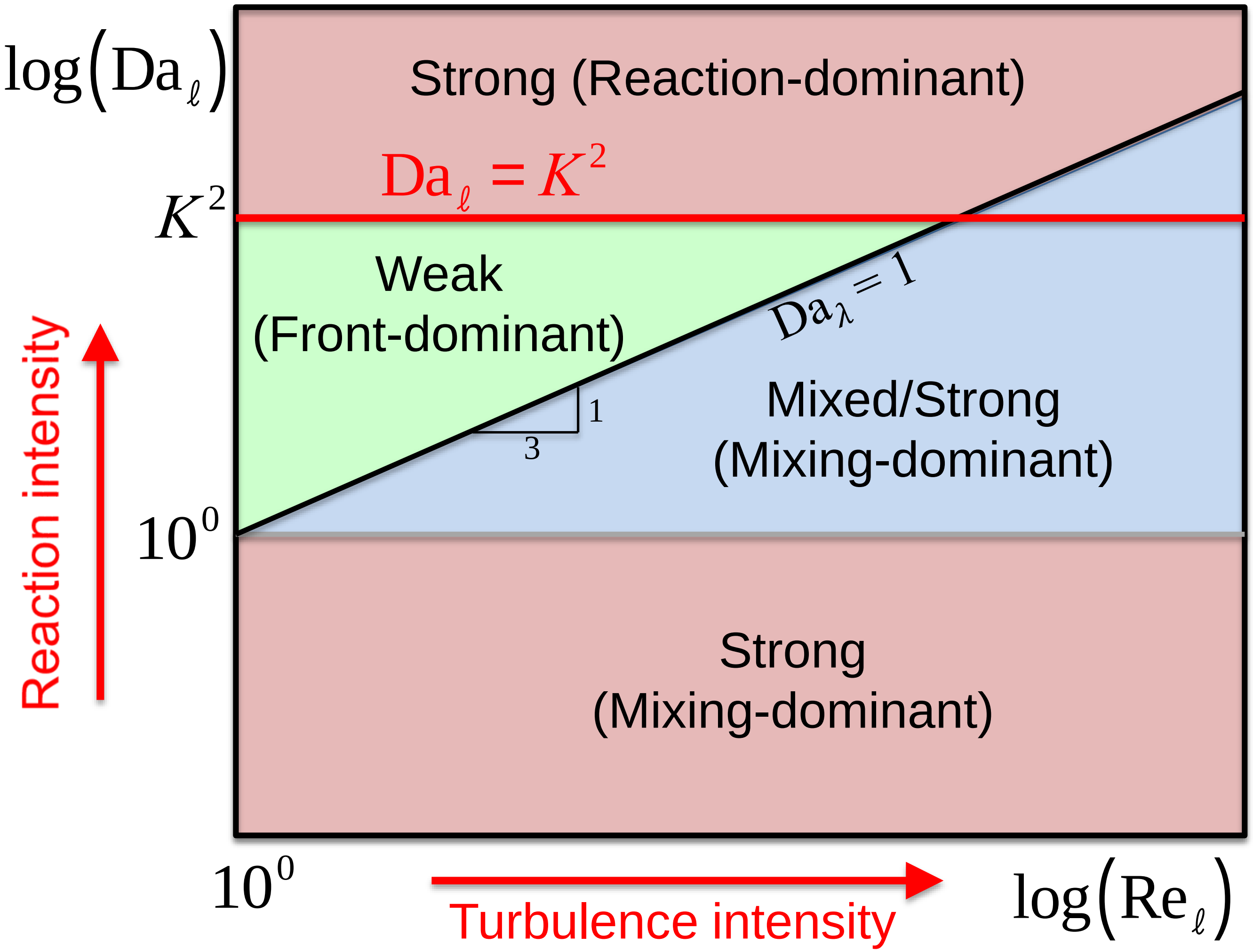
# The Regime Diagram




$$\mathrm{Da}_\ell = \frac{t_\ell}{t_{ig}} = \frac{\ell / u'}{t_{\mathrm{ig}}}$$

$$\mathrm{Da}_\lambda = \frac{t_\lambda}{t_{\mathrm{ig}}} = \mathrm{Da}_\ell \, \mathrm{Re}_\ell^{-1/3}$$

$$K = b\left(\frac{T'}{t_f}\right)\left(\frac{dt_{\mathrm{ig}}}{dT}\right)$$

# Experimental Data on the Diagram

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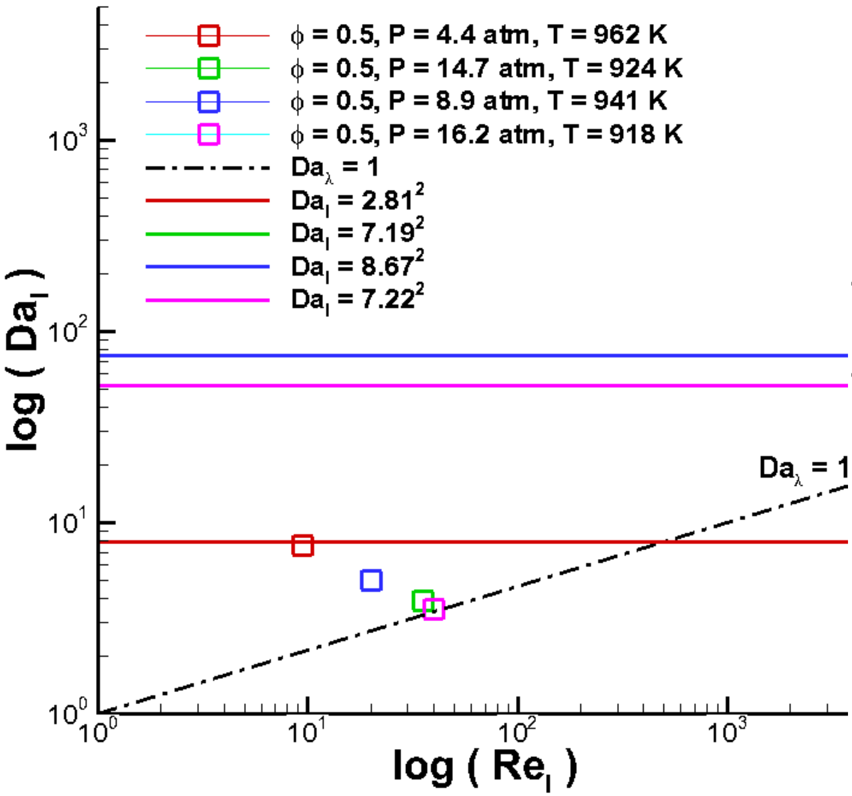
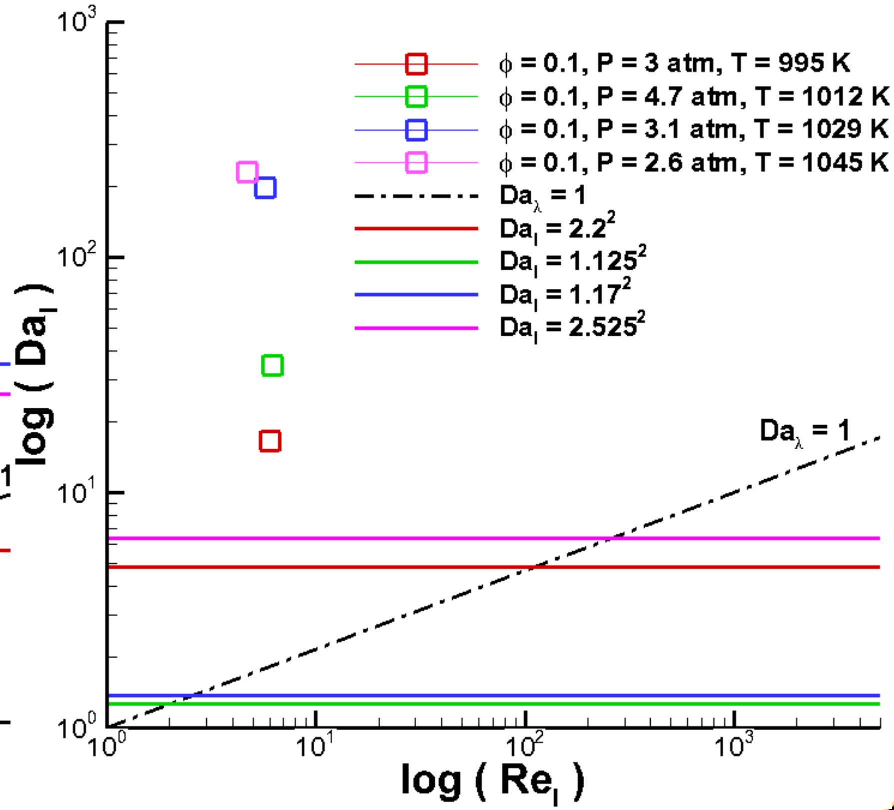
Data from Mansfield & Wooldridge (2014)

## Weak Ignition Cases




## Strong Ignition Cases



# Remarks/Reflections

- The Sankaran-Zeldovich criterion combines both thermochemical property ($K$) of the mixture and the flow/scalar field conditions ($Da_\ell$, $Re_\ell$).
- The ignition sensitivity is more than just a characteristic time scale, thus a simple Damköhler number-based (based on time scales only) characterization is not sufficient to describe the phenomena.
- High-$K$ mixtures are more susceptible to weak ignition, which happens at low temperatures for hydrogen/oxygen mixtures. Therefore, the observed ignition advancement for syngas at low temperatures may be attributed to the weak ignition behavior.
- On the other hand, for higher hydrocarbon fuels with NTC behavior, there is a broad range of intermediate temperature conditions where $K$ is low (or negative), where the system will be more susceptible to strong ignition. Further studies are needed for the weak ignition behavior for fuels at NTC conditions (Gupta et al., PROCI 2013).