# Robust, Reliable Low Emission Gas Turbine Combustion of High-Hydrogen-Content Fuels

## *Prediction of Auto-ignition Regimes in the Presence of Temperature Inhomogeneities and Turbulence*

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# Outline

1) Motivation

2) Auto-ignition regime prediction (1D numerical study)

3) Regime criteria for turbulent ignition

4) Turbulent ignition regime diagram

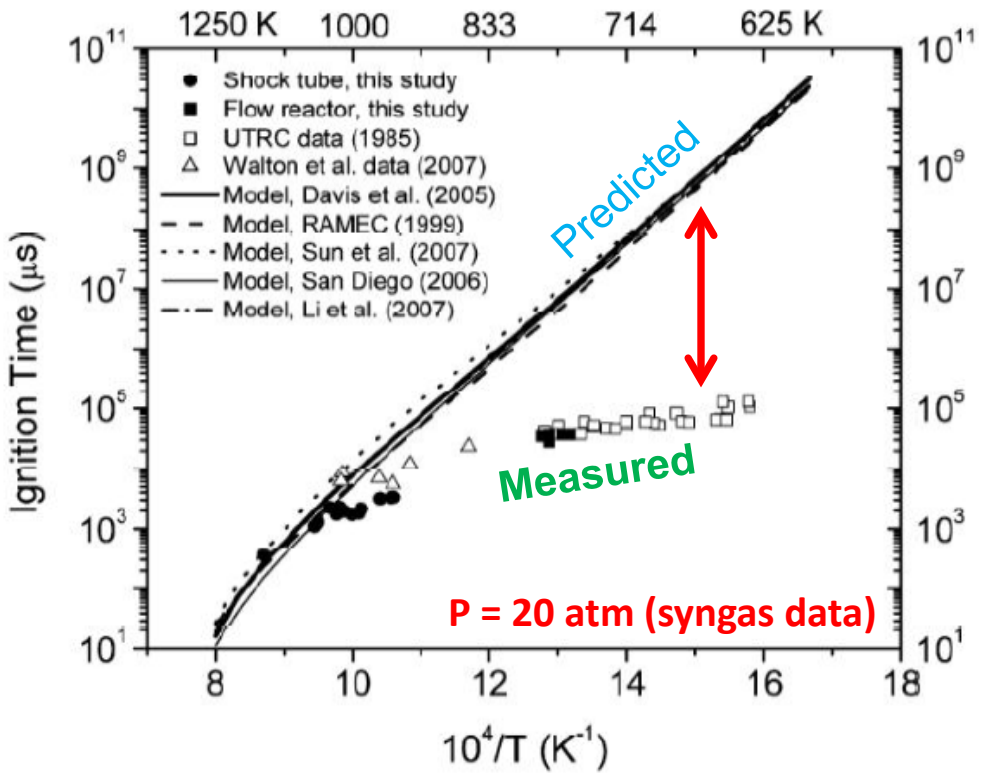
5) Validation of regime diagram (2D DNS)

6) Conclusions and future work

# Motivation

## *Discrepancy in ignition delay times*

- Combustion under typical gas turbine operating conditions of high pressures (up to 30 atm) and low/intermediate temperatures (T < 1000 K) is not sufficiently well understood.



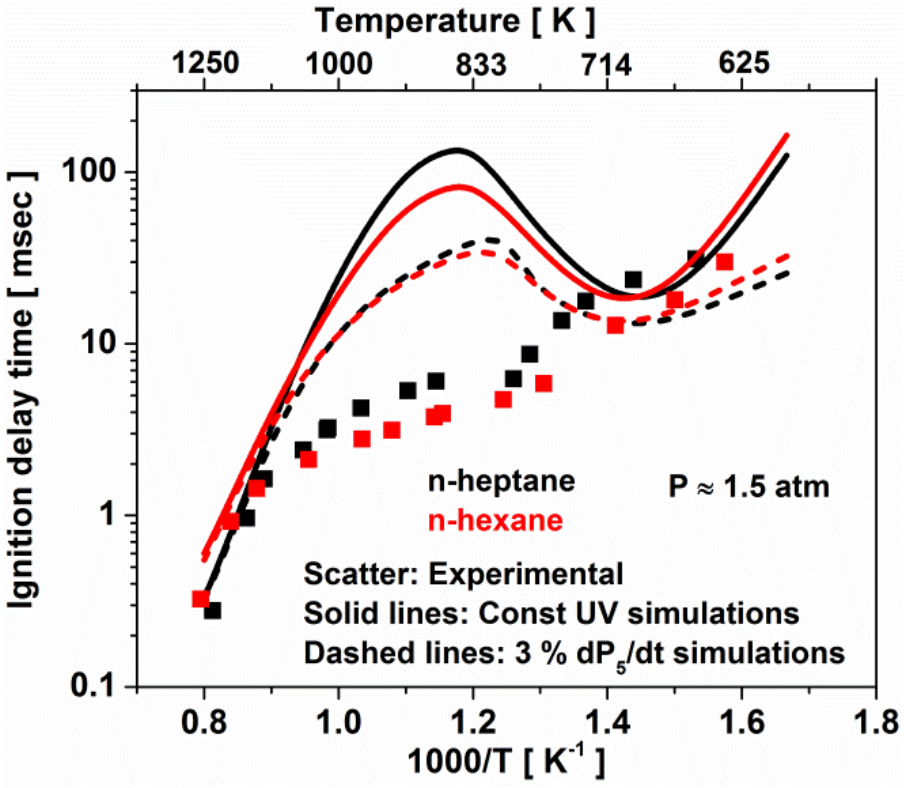

Petersen et al., 2007

- Marked discrepancy in ignition delay between measurements and 0D chemical kinetic modeling.

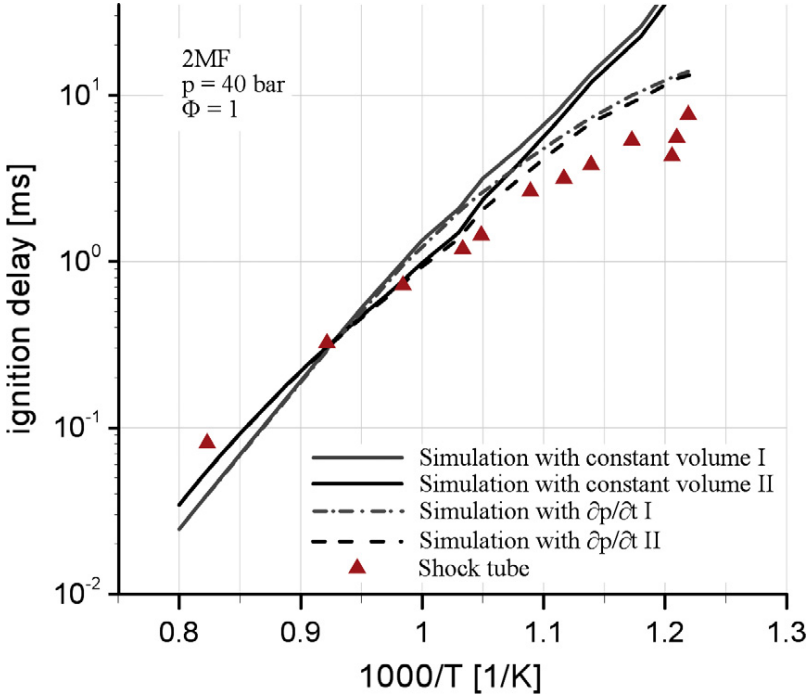
**Need to investigate and characterize auto-ignition behaviors**

# Motivation

## *Discrepancy in ignition delay times*




Javed et al., KAUST Low Pressure Shock Tube



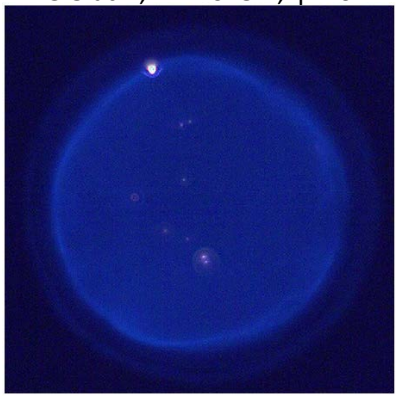

Uygun, Ishihara, Olivier, C&F 2014

# Motivation

## *"Strong" and "weak" ignition regimes*

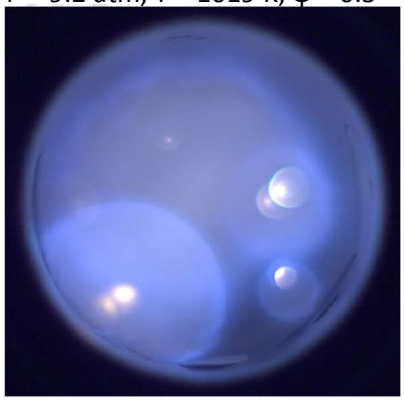
**Mansfield and Wooldridge, C&F 2014**

P = 3.3 atm, T = 1043 K, ϕ = 0.1

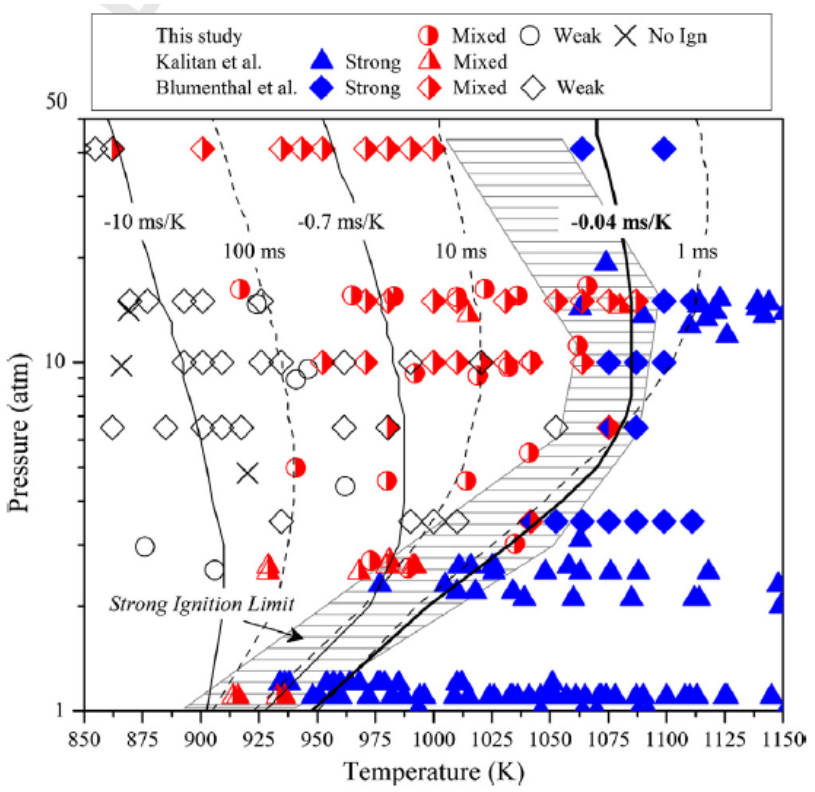


**Volumetric ignition (strong)**

P = 9.2 atm, T = 1019 K, ϕ = 0.5



**Localized ignition sites + deflagrative ignition fronts (weak)**



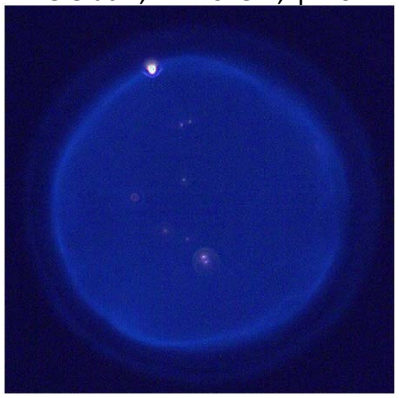

- Transition from strong to weak ignition behavior was observed as the initial mean temperature was lowered.
- Weak ignition at lower temperature conditions was attributed to the higher sensitivity of ignition delay to temperature perturbations, $\partial \tau_{ig} / \partial T$.

# Motivation

## *"Strong" and "weak" ignition regimes*

**Mansfield and Wooldridge, C&F 2014**

P = 3.3 atm, T = 1043 K, ϕ = 0.1



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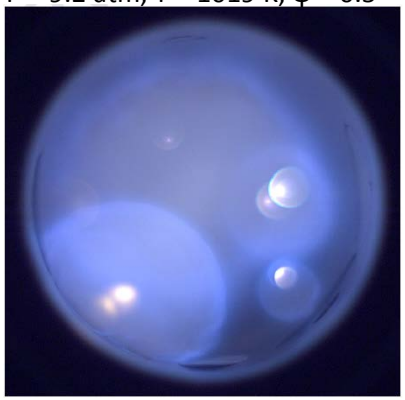
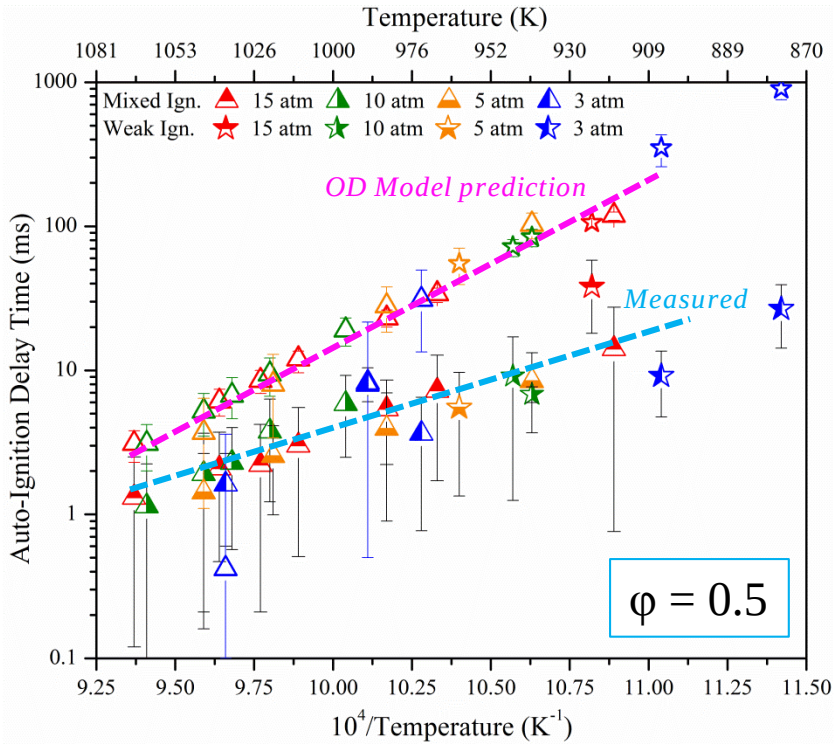


**Localized ignition sites + deflagrative ignition fronts (weak)**




- Overall ignition was considerably advanced in weak ignition scenarios.

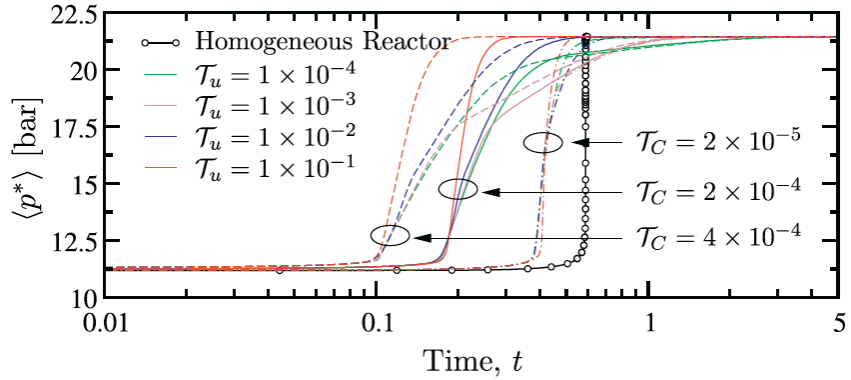
**HOW TO PREDICT STRONG AND WEAK IGNITION REGIMES *a priori* ??**

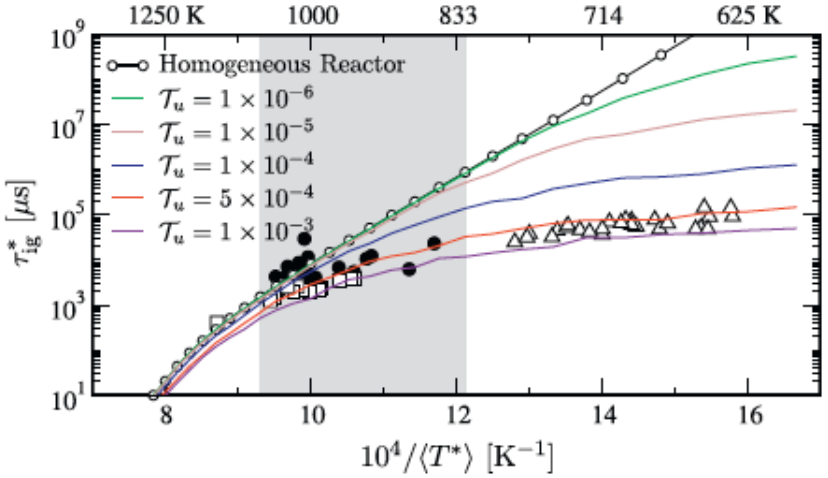
# Motivation

## *Turbulence-chemistry interaction*

Ihme, C&F 2012

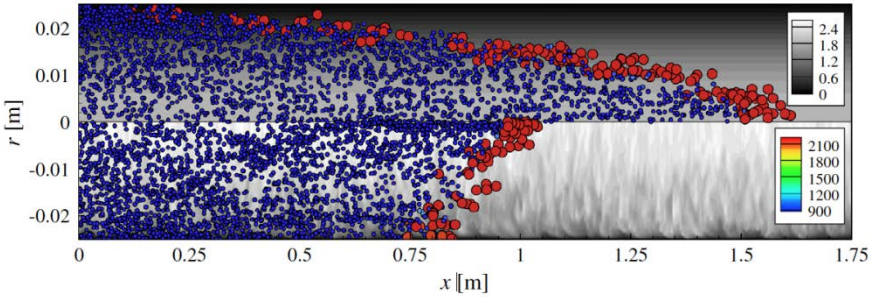
0D model prediction

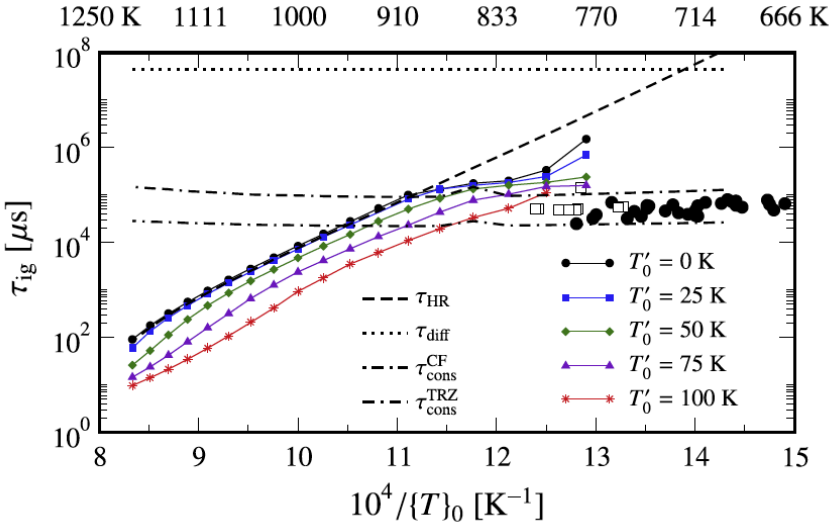



Wu & Ihme, C&F 2014

Lagrangian model prediction



# Objectives

1) To identify and characterize syngas auto-ignition regimes in the presence of thermal inhomogeneities

2) To predict the transition between “strong” and “weak” ignition phenomena

# Auto-ignition regime prediction

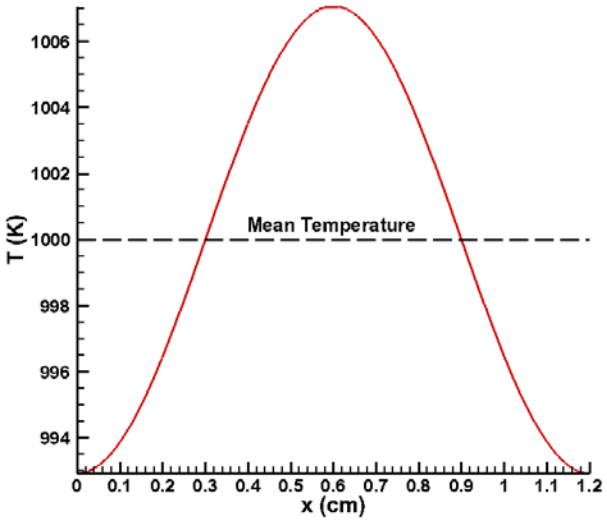
## *1D numerical study: Model setup*

*Pal et al., CTM (2015)*

- High fidelity one-dimensional numerical simulations were performed using S3D DNS code.
- Detailed $H_2$/CO mechanism with 12 species and 33 chemical reactions was employed [Li et al., 2007]. Detailed thermodynamic and mixture-averaged transport properties were incorporated.
- The following range of thermo-chemical states were considered in study:

  - **T = 850 – 1100 K**
  - **P = 10 – 20 atm**
  - **φ = 0.5 ($H_2$ : CO molar ratio = 0.7 : 1)**

- Periodic boundary conditions were imposed to enforce a fixed volume, thereby incorporating compression heating and pressure-rise of reactants due to ignition. Initial flow conditions were quiescent.
- A fine grid resolution of 4.7 μm was used to resolve the thin propagating reaction fronts.



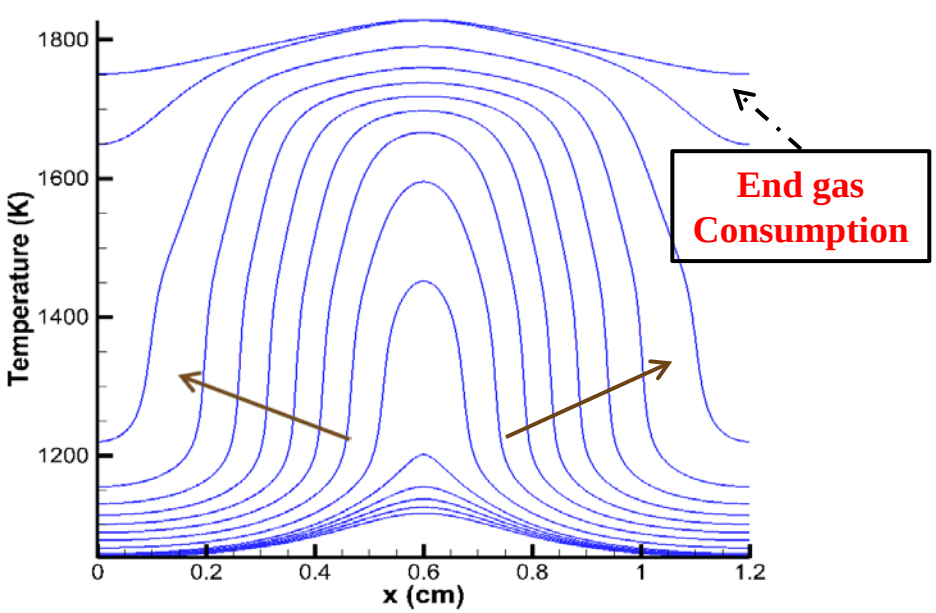

Initial T profile

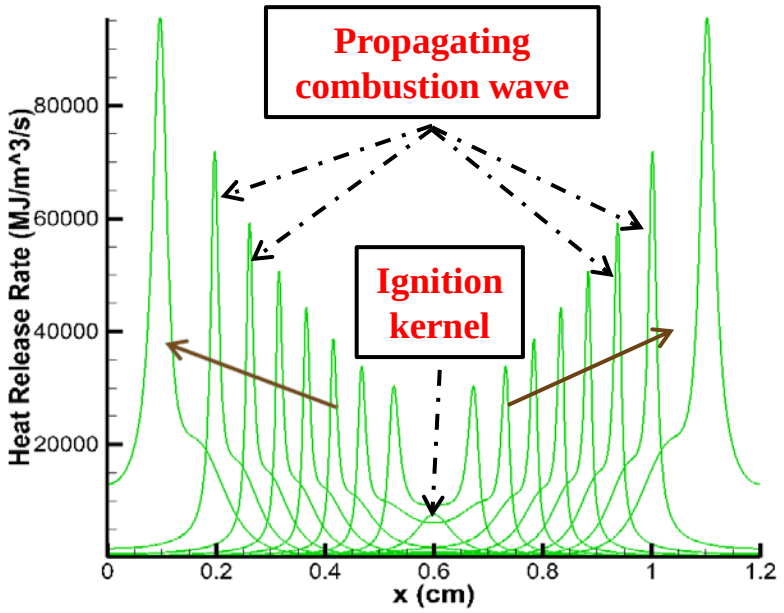
# Auto-ignition regime prediction

## *1D numerical study: Ignition front propagation*

*Pal et al., CTM (2015)*

**P = 10 atm, φ = 0.5, $T_i$ = 1050 K, $T_{rms}$ = 10 K**




- An ignition kernel first develops at the location of highest temperature. Subsequently, combustion waves emanate from this location. As fronts propagate, the remaining charge is heated by compression, thereby accelerating the ignition of the end-gas mixture.

**What is the nature of the propagating front?**

**Deflagration versus spontaneous ignition**

# Auto-ignition regime prediction

## *1D numerical study*

### Classification of Reaction Front Regime

*Pal et al., CTM (2015)*

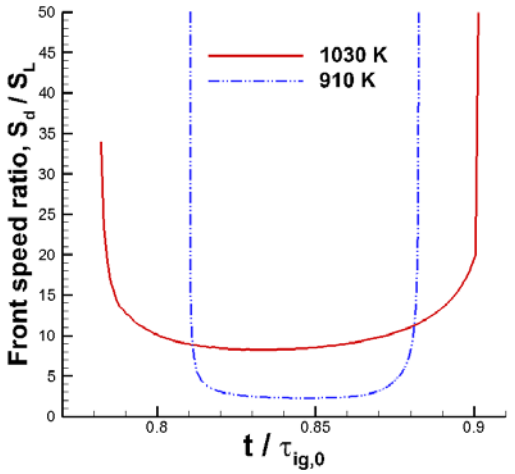
- **Front propagation speed**

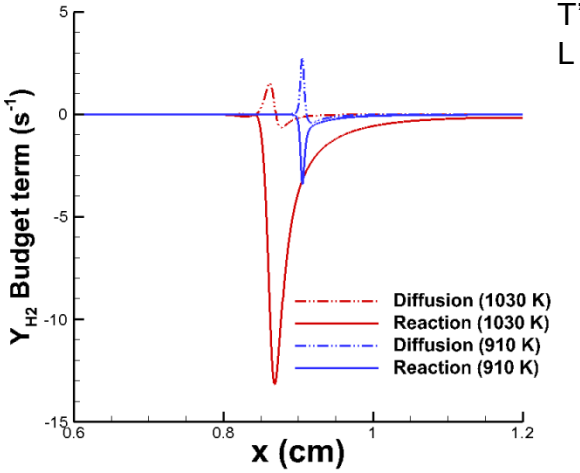
$$S_d = \frac{1}{\rho_u \,|\nabla Y_{H_2}|}\left(\dot{\omega}_{H_2} - \frac{\partial}{\partial x_j}\left(\rho Y_{H_2} V_{j,H_2}\right)\right)$$

- **Reaction/Diffusion budget**

$$Da_{fr} = \frac{\max(\dot{\omega}_{H_2})}{\max(\nabla.(-\rho D_{H_2} \nabla Y_{H_2}))}$$

- Spontaneous ignition front (strong ignition) occurs at high mean temperature and deflagrative front (weak ignition) occurs at low mean temperature.
- Final thermal runaway occurs earlier at lower mean temperature.




$P_i$ = 20 atm
$\varphi$ = 0.5
T' = 10 K
L = 1.2 cm

# Auto-ignition regime prediction
## 1) *Zel'dovich-Sankaran criterion*

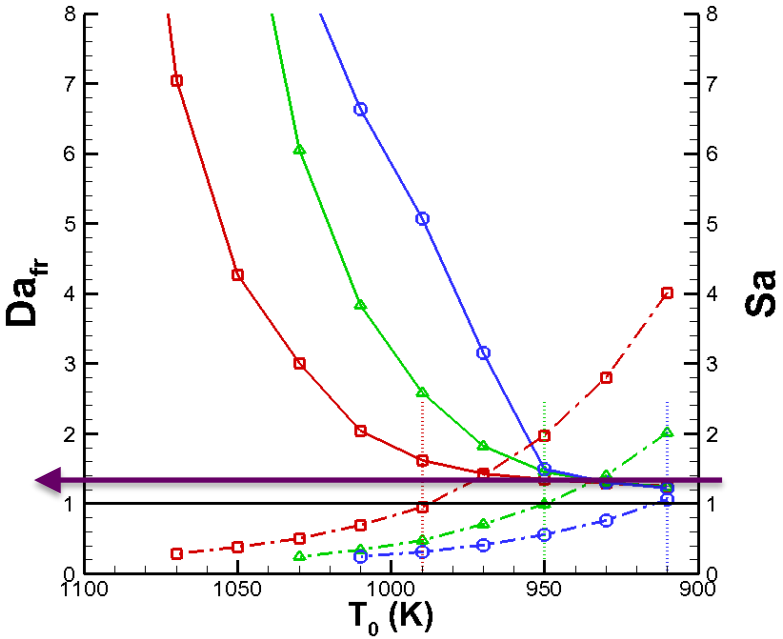
*Pal et al., CTM (2015)*

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} = \beta S_L \left( \frac{d\tau_{\mathrm{ig},0}}{dT} \right) \left( \frac{dT_0}{dx} \right) \quad (\beta \approx 0.5)$$

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

- Sa serves as an *a priori* criterion for weak versus strong ignition, and describes the role of chemical kinetics, thermophysical properties and device-dependent thermal characteristics on auto-ignition behavior.

| Set # | $P_0$ (atm) | $T'$ (K) | $L$ (cm) |
|---|---|---|---|
| 1 | 20 | 10 | 1.2 |
| 2 | 10 | 10 | 1.2 |
| 3 | 10 | 10 | 2.4 |




**Sa = 1 correlates well with $Da_{fr}$ ≈ 1.4**

# Auto-ignition regime prediction

## 2) *Scalar mixing criterion*

*Pal et al., CTM (2015)*

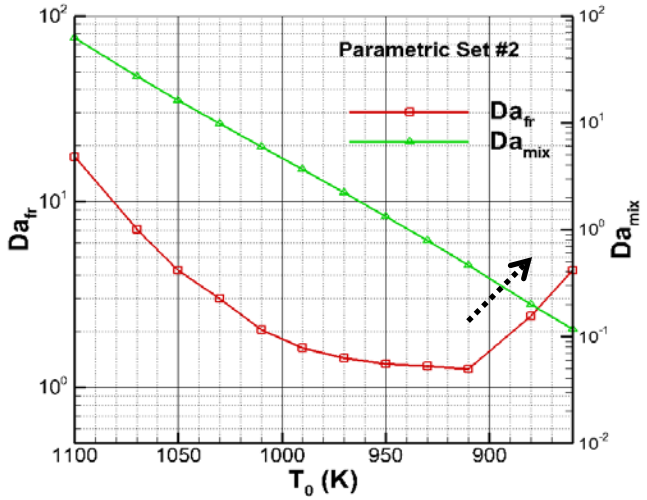
- Passive scalar dissipation modifies the statistics of the pre-ignition temperature field, by dissipating the fluctuations before any significant reaction occurs.

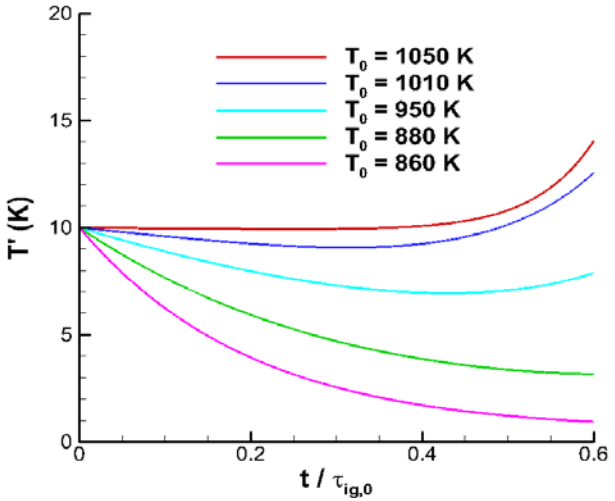
$$\tau_{mix} = \frac{T''^2}{2\alpha_0 \left|\nabla T_0\right|^2}$$

$$\mathrm{Da}_{mix} = \tau_{mix} / \tau_{ig,0} < O(1)$$

⇩

Strong Ignition



# *Next steps…*

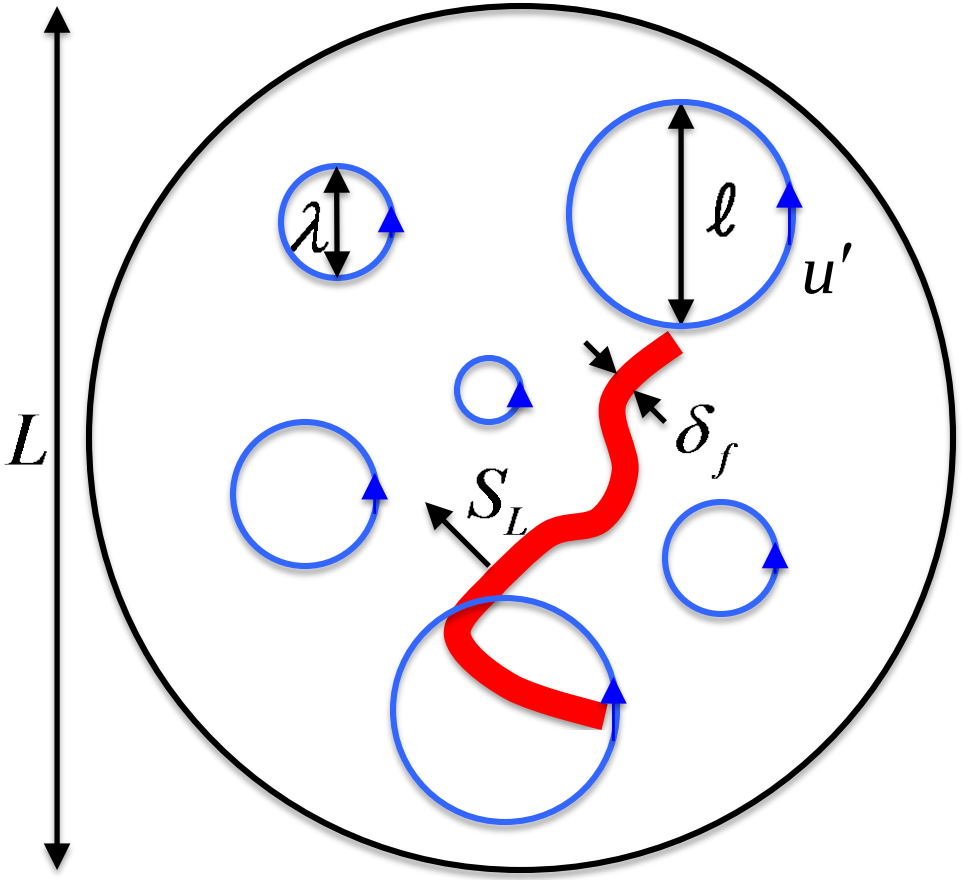
1) **Extend the auto-ignition regime criteria to turbulent flow conditions**

2) **Validate the turbulent ignition regime criteria**

# Turbulent ignition regime criteria

## *Schematic of scales*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*




$L$ : chamber length (not considered)

$\ell$ : integral eddy scale

$\lambda$ : Taylor microscale

$\delta_f$ : Deflagration flame thickness

$S_L$ : Laminar flame speed

Homogeneous turbulence:

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

# Turbulent ignition regime criteria

## *Assumptions and hypotheses*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*

- Scales of temperature and velocity fluctuations are comparable.

- 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).

# Turbulent ignition regime criteria

## 1) *Sankaran number formulation*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*

### Turbulent Sankaran (Zel'dovich) Number

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

where

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

hence

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

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

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

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

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

# Turbulent ignition regime criteria

## 1) *Sankaran number formulation*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*

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

where

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

$$\mathrm{Da}_\ell = \frac{\tau_\ell}{\tau_{ig}} \quad \text{(Integral Da)}$$

**Modified ignition criterion for turbulent combustion:**

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

# Turbulent ignition regime criteria

## 2) *Scalar mixing criterion*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*

$$\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{\mathrm{ig}}}$$

Mixing Da – based on mixing (Taylor) scale eddies

where the mixing time and scale is determined by

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

$T'$: RMS temperature fluctuation

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

$$\tau_{\lambda_T} = \tau_\lambda; \quad \lambda_T = \lambda$$

It follows that $\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{\mathrm{ig}}} = \frac{\tau_\lambda}{\tau_{\mathrm{ig}}} = \frac{\tau_\ell}{\tau_{\mathrm{ig}}}\frac{\tau_\lambda}{\tau_\ell} = \mathrm{Da}_\ell \mathrm{Re}_\ell^{-1/3}$

$$\mathrm{Re}_\ell = \frac{u'\ell}{\nu}$$

# Turbulent ignition regime criteria

## 2) *Scalar mixing criterion*

*Im, Pal, Wooldridge, Mansfield, CST (2015)*

Thermal fluctuations will dissipate before the front forms if

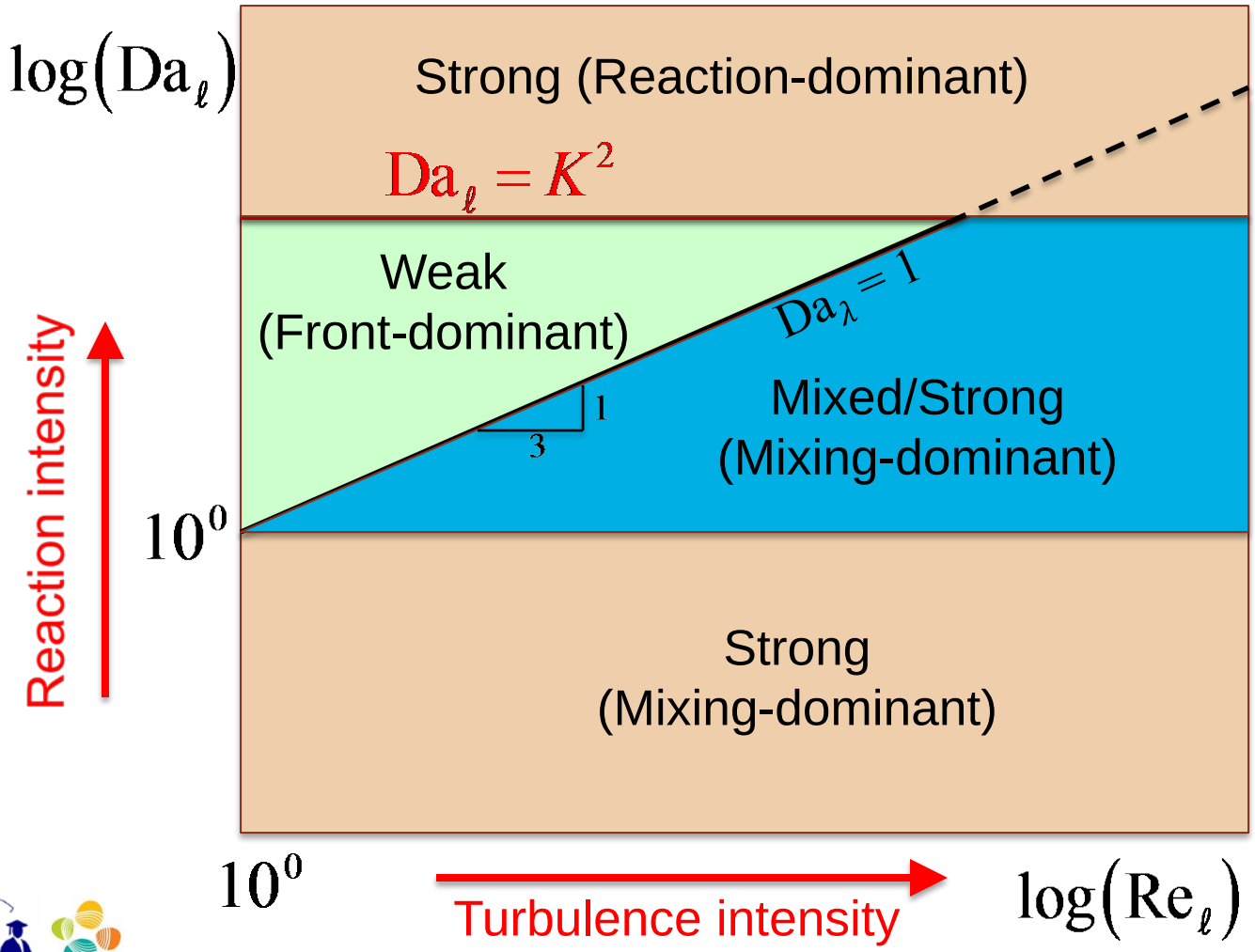
$$\mathrm{Da}_\lambda = \mathrm{Da}_\ell \, \mathrm{Re}_\ell^{-1/3}$$

$$\begin{cases} \mathrm{Da}_\lambda > 1 & \text{Weak ignition possible} \\ \mathrm{Da}_\lambda < 1 & \text{Mixed/Strong (mixing-dominant)} \end{cases}$$

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

# Turbulent ignition regime diagram

*Im, Pal, Wooldridge, Mansfield, CST (2015)*




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

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

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

# Regime diagram validation

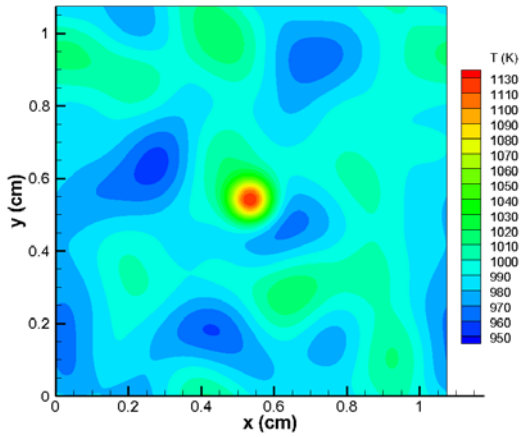
## *2D DNS of Syngas auto-ignition*

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

| Case | $T_0$ (K) | $\tau_{ig}$ (ms) | $T'$ (K) | $K^2$ | $\ell$ (mm) | $u'$ (m/s) | $\tau_\ell$ (ms) | $Da_\ell$ | $Re_\ell$ | $Da_\lambda$ | $\frac{\tau_{HRR\_max}}{\tau_{ig}}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| A | 990 | 25.77 | 15 | 4.05 | 4.3 | 0.05 | 86.0 | 3.34 | 35.24 | 1.02 | 50 |
| B | 1100 | 2.07 | 15 | 2.51 | 4.3 | 0.05 | 86.0 | 41.6 | 29.40 | 13.5 | 82 |
| C | 990 | 25.77 | 15 | 4.05 | 4.3 | 1.50 | 2.87 | 0.11 | 1057.4 | 0.01 | 93 |
| D | 1100 | 2.07 | 15 | 2.51 | 6.0 | 0.2 | 30 | 14.5 | 164 | 2.65 | 87 |
| E | 990 | 25.77 | 15 | 4.05 | 6.0 | 0.2 | 30 | 1.16 | 197 | 0.2 | 55 |
| F | 970 | 41.26 | 15 | 4.41 | 6.0 | 0.05 | 120 | 2.91 | 50 | 0.8 | 56 |
| G | 1020 | 12.7 | 15 | 3.28 | 4.0 | 0.3 | 13.33 | 1.05 | 185 | 0.2 | 57 |

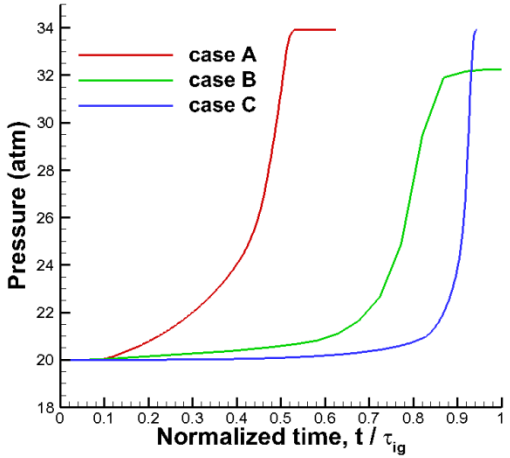
- Periodic boundary conditions on all sides
- Passot-Pouquet turbulent kinetic energy spectrum
- Uncorrelated temperature and velocity fields
- Hot spot superimposed on the random T field at the center of the domain
- Syngas/air detailed chemical kinetic mechanism with 12 species and 33 reactions (*Li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

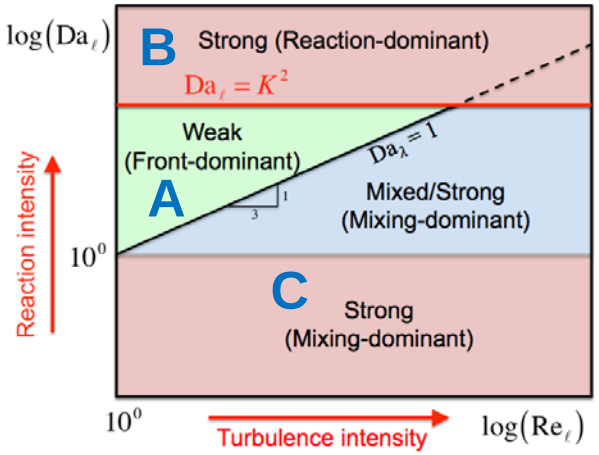
Case A (Initial T profile)



# Regime diagram validation

## *2D DNS: Evolution of temperature field*

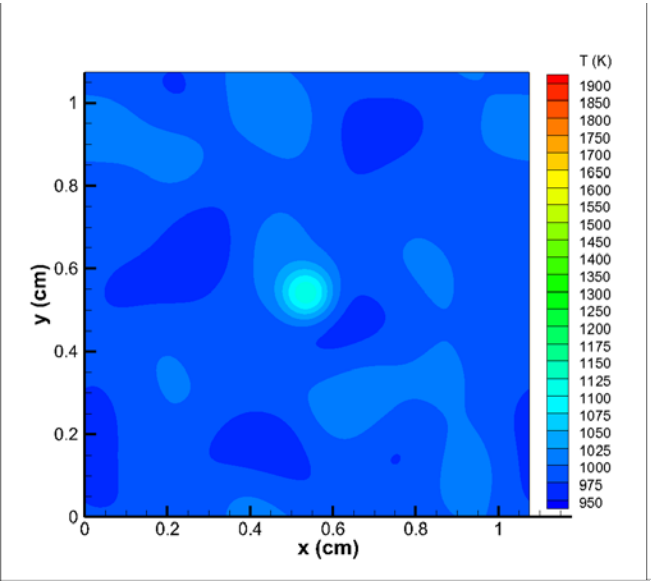


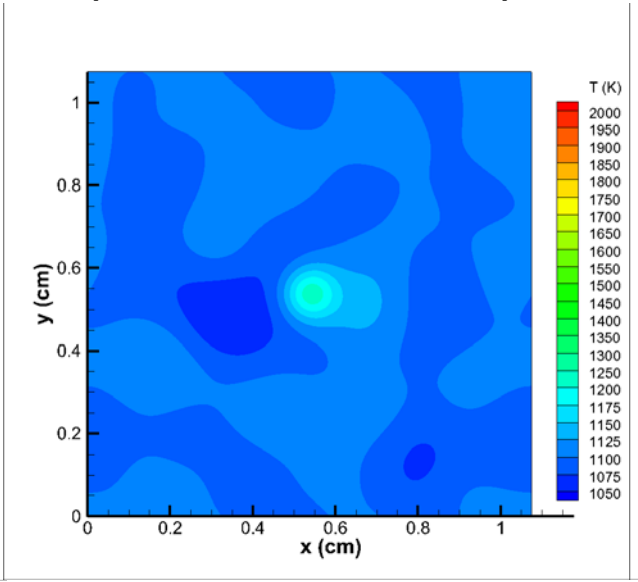



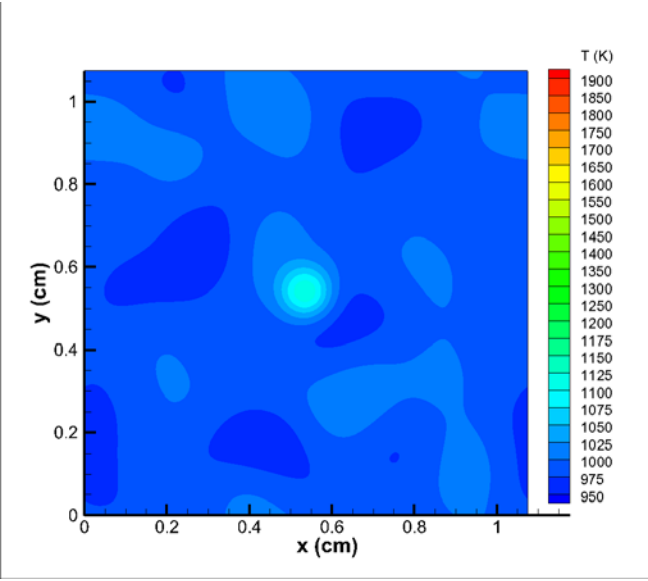

A. Weak Ignition

B. Strong Ignition (Reaction-dominant)

C. Strong Ignition (Mixing-dominant)



# Conclusions & future work

- In the present study, auto-ignition regimes in the presence of thermal inhomogeneities are investigated at high-pressure, low-temperature conditions.
- Non-dimensional criteria based on the Sankaran number and mixing Damkohler number are identified to identify the ‘strong’ and ‘weak’ ignition regimes.
- The ignition regime criteria are further extended to turbulent flow conditions based on scaling analysis, leading to a turbulent ignition regime diagram.
- 2D DNS of syngas auto-ignition in the presence of thermal and turbulent fluctuations are performed for conditions representative of different regions of the regime diagram.
- Analysis of pressure/heat release and evolution of the temperature fields indicates that the observed auto-ignition behaviors are consistent with predictions of the proposed ignition regime diagram.

- Future work (work in progress):
  - Detailed post-processing/analysis of the simulation data using CSP
  - Validation of the auto-ignition regime criteria for higher hydrocarbon fuels at both NTC and non-NTC conditions
  - Extension of the auto-ignition regime criteria to incorporate mixture stratification
  - Application of the regime diagram to practical combustion devices such as engines


Thank You