King Abdullah University of Science and Technology KAUST

Computational Studies of Syngas Auto-ignition with Thermal Inhomogeneities

Pinaki Pal, Ph.D. Candidate
Andrew B. Mansfield, Ph.D. Candidate
Margaret S. Wooldridge, Professor
University of Michigan, Ann Arbor, MI, USA

Hong G. Im, Professor
Clean Combustion Research Center
King Abdullah University of Science and Technology (KAUST)
Thuwal, Saudi Arabia

“Weak” versus “Strong” Ignition

King Abdullah University of Science and Technology

KAUST

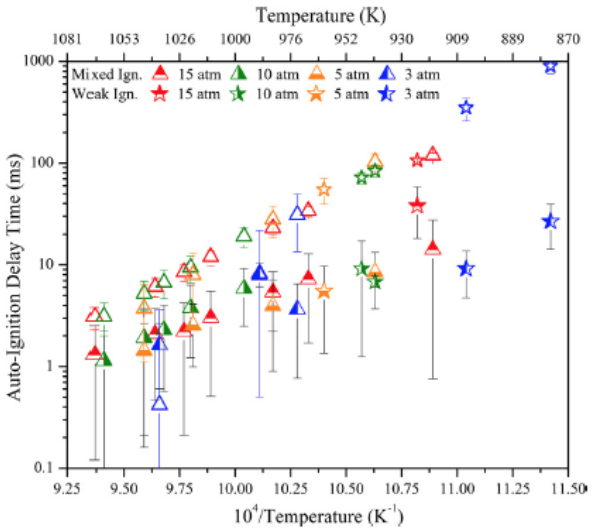
Mansfield and Wooldridge, C&F 2014

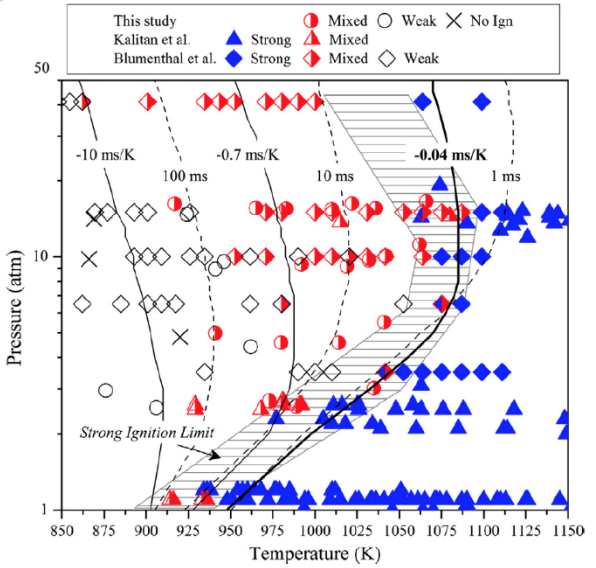
P = 3.3 atm, T = 1043 K, φ = 0.1

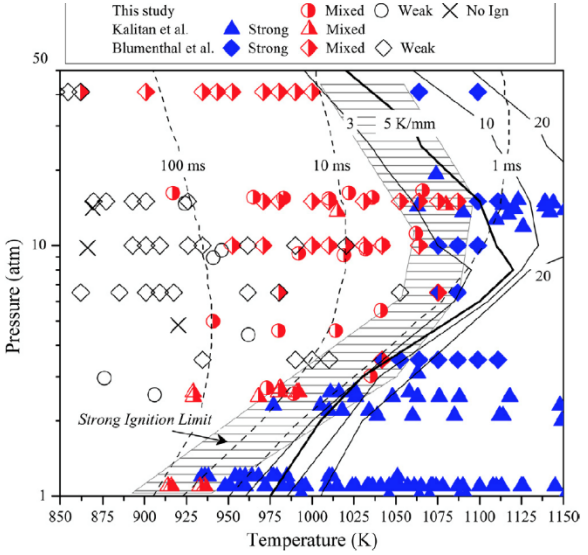
P = 9.2 atm, T = 1019 K, φ = 0.5

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

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







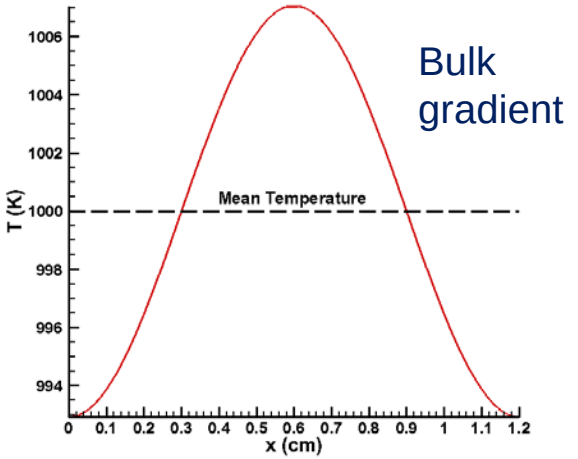
1D Model Configuration

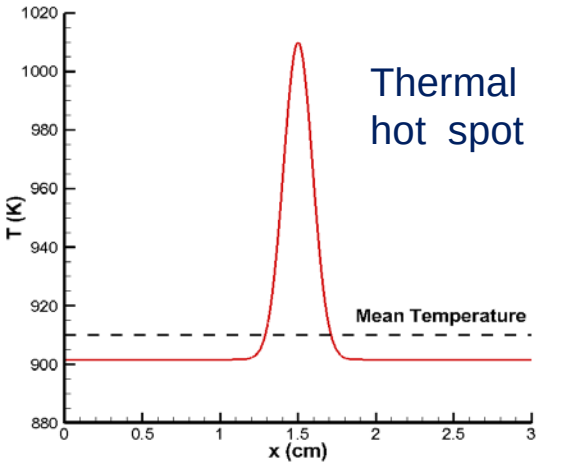
King Abdullah University of Science and Technology KAUST

- High fidelity one-dimensional numerical simulations are performed using S3D DNS code.
- Detailed H_2/CO mechanism with 12 species and 33 chemical reactions is employed *[Li et al., 2007].* Detailed thermodynamic and mixture-averaged transport properties are incorporated.
- Following range of thermo-chemical states are considered for parametric study:

  - **T = 850 – 1100 K**
  - **P = 3 – 20 atm**
  - **φ = 0.1, 0.5 (H_2 : CO molar ratio = 0.7 : 1)**

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



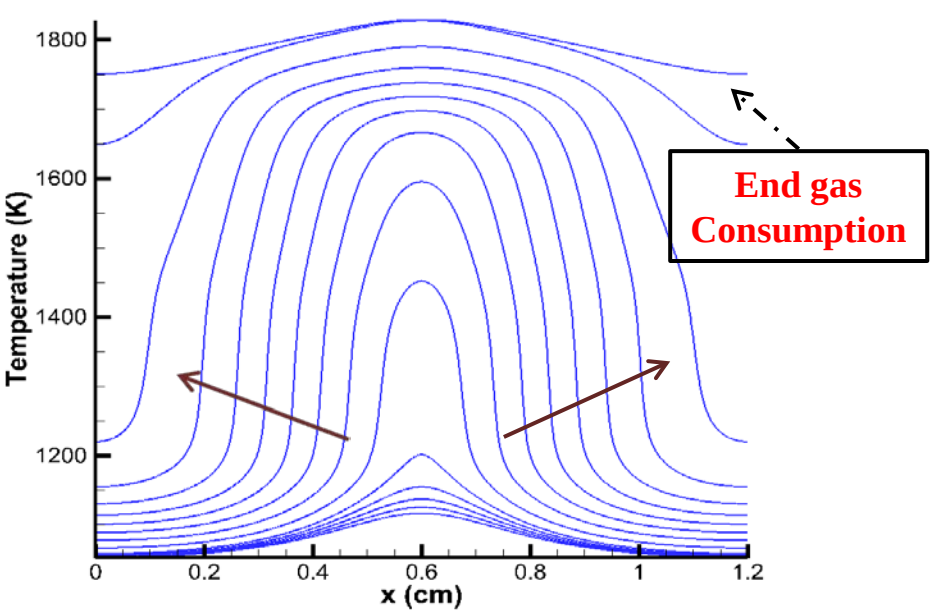


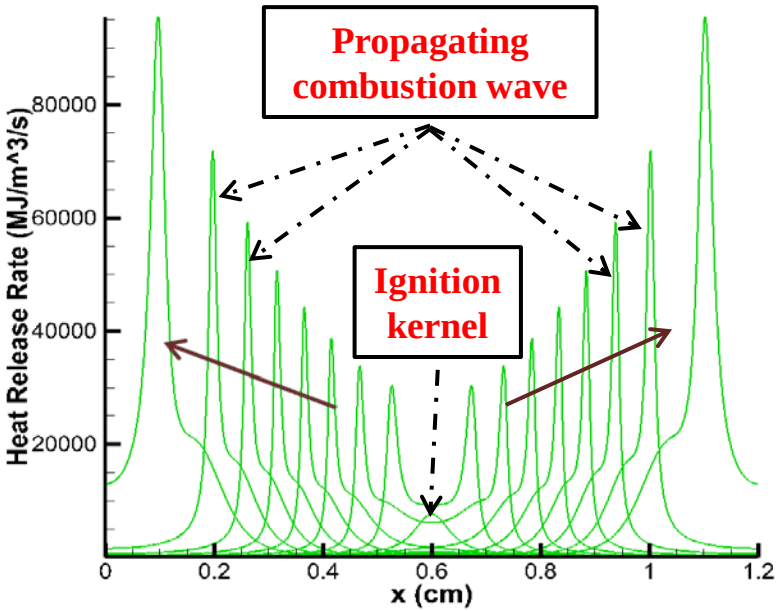
Evolution of Ignition Front Development and Propagation

King Abdullah University of Science and Technology

KAUST

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 gets heated by compression, accelerating the ignition of the end-gas mixture.

What is the nature of the propagating front?
; Deflagration versus Spontaneous

Effect of Bulk Temperature Gradient

King Abdullah University of Science and Technology KAUST

Classification of Ignition Regimes

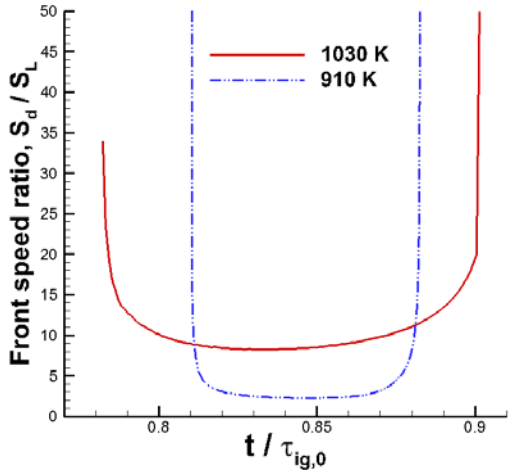
- **Front propagation speed**

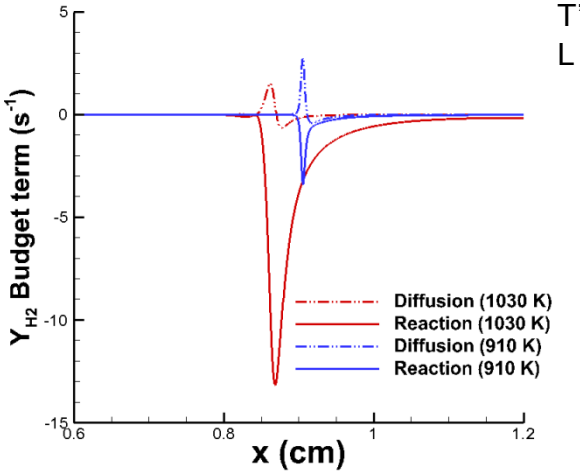
$$S_d = \frac{1}{\rho_u |\nabla Y_{H_2}|}\left(\dot{\omega}_{H_2} - \frac{\partial}{\partial x_j}\left(\rho Y_{H_2} V_{j,H_2}\right)\right)$$

- **Front Damkohler number**

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

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





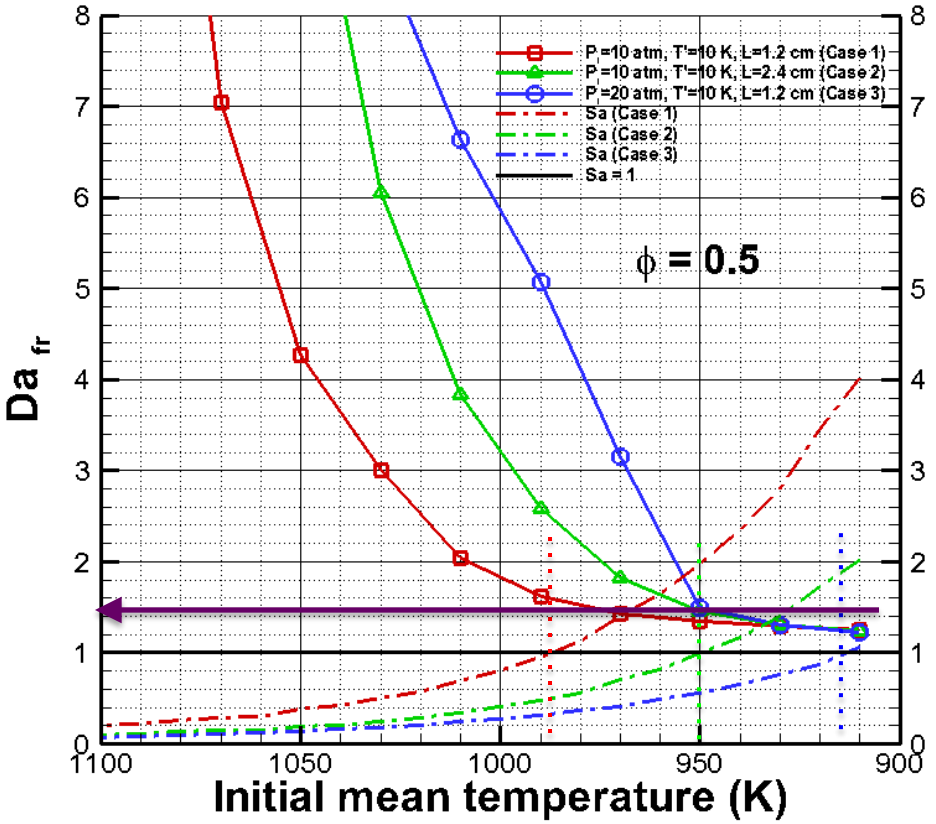
P_i = 20 atm
φ = 0.5
T' = 10 K
L = 1.2 cm

Equality of Sa and Da_{fr}

King Abdullah University of Science and Technology

KAUST

Parametric study



- **The Sankaran (Zeldovich) Criterion (2006)**

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} < 1$$: Strong ignition

$$\beta = 0.5$$

$$S_{sp} = \left| \nabla T \cdot \frac{d\tau_{ig}}{dT} \right|^{-1}$$

Sa

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

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

Rapid Mixing Scenario

King Abdullah University of Science and Technology KAUST

Role of passive scalar mixing

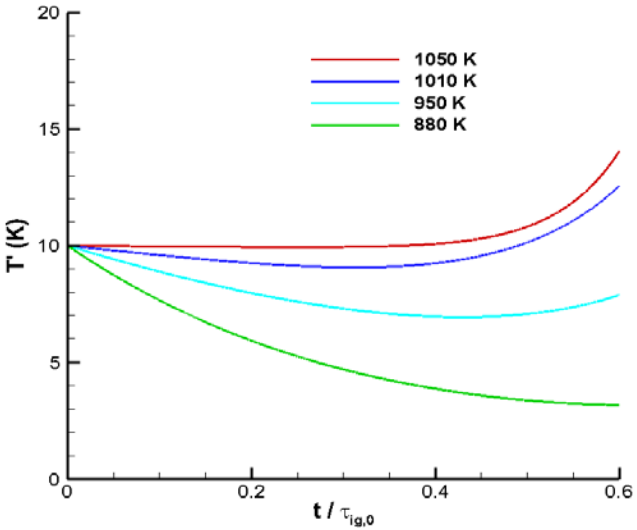
- Passive scalar dissipation modifies the statistics of the pre-ignition temperature field, by dissipating the fluctuations before any significant reaction occurs.

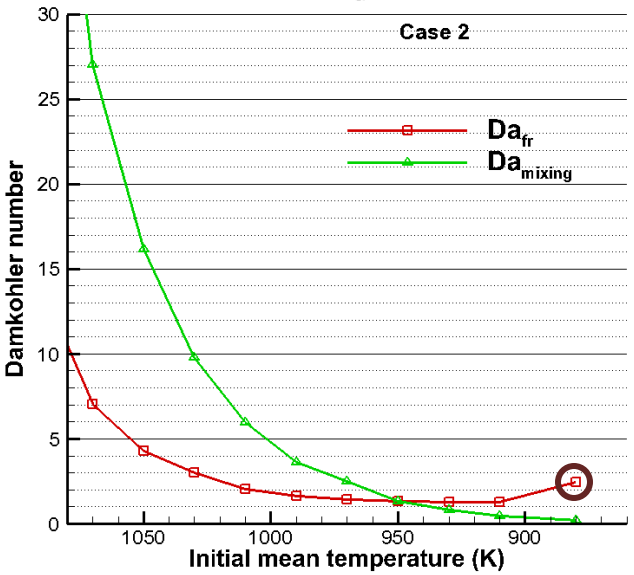
- A time scale associated with passive mixing can be defined as

$$\tau_{mix} = \frac{T_{rms}^2}{2\alpha |\nabla T|^2}$$

- At sufficiently low temperatures, mixing has more pronounced effect in shifting the ignition behavior from deflagrative back to spontaneous when

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





Hot Spot Autoignition

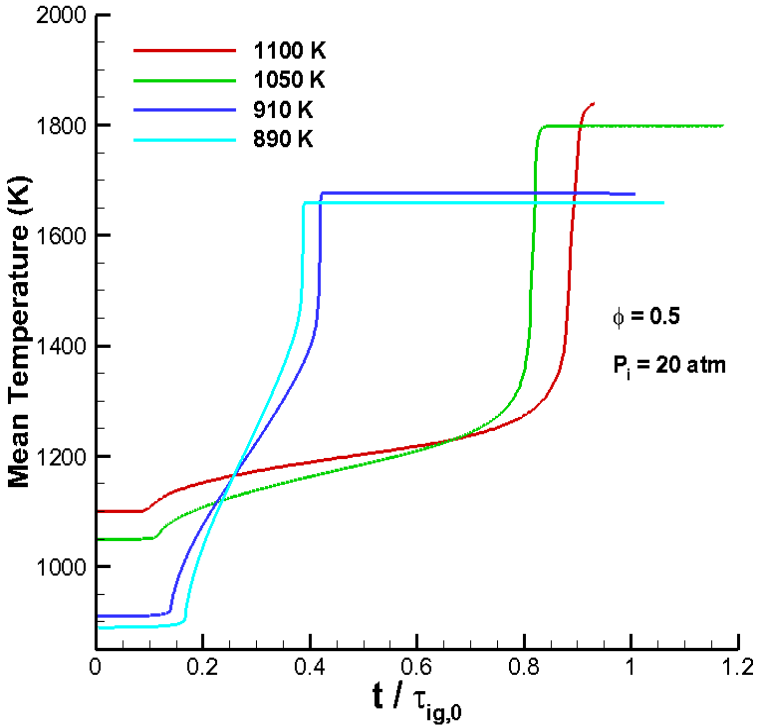
King Abdullah University of Science and Technology KAUST

Variation of initial mean temperature

- Sankaran number (Sa) is defined in terms of the RMS T fluctuation and the domain size.

Initial mean T (K)	Sa
1100	0.06
1050	0.12
910	0.96
890	1.82

- As Sa increases, the end gas auto-ignition due to compression effect of the front is advanced, resulting in increasingly weak ignition behavior.



Constant hot spot strength
peak ΔT = 100 K

Hot Spot Autoignition (2)

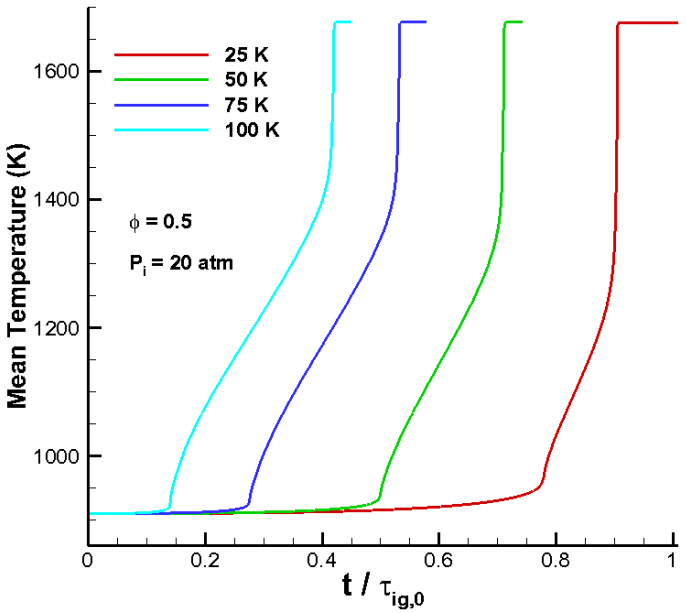
King Abdullah University of Science and Technology KAUST

Variation of hot spot strength

- Sankaran number (Sa) is defined in terms of the RMS T fluctuation and the domain size.

peak ΔT (K)	Sa
25	0.24
50	0.48
75	0.72
100	0.96

- The trend of increased compression heating of the end gas and faster thermal runaway with increase in the hot spot strength is also captured by Sa.

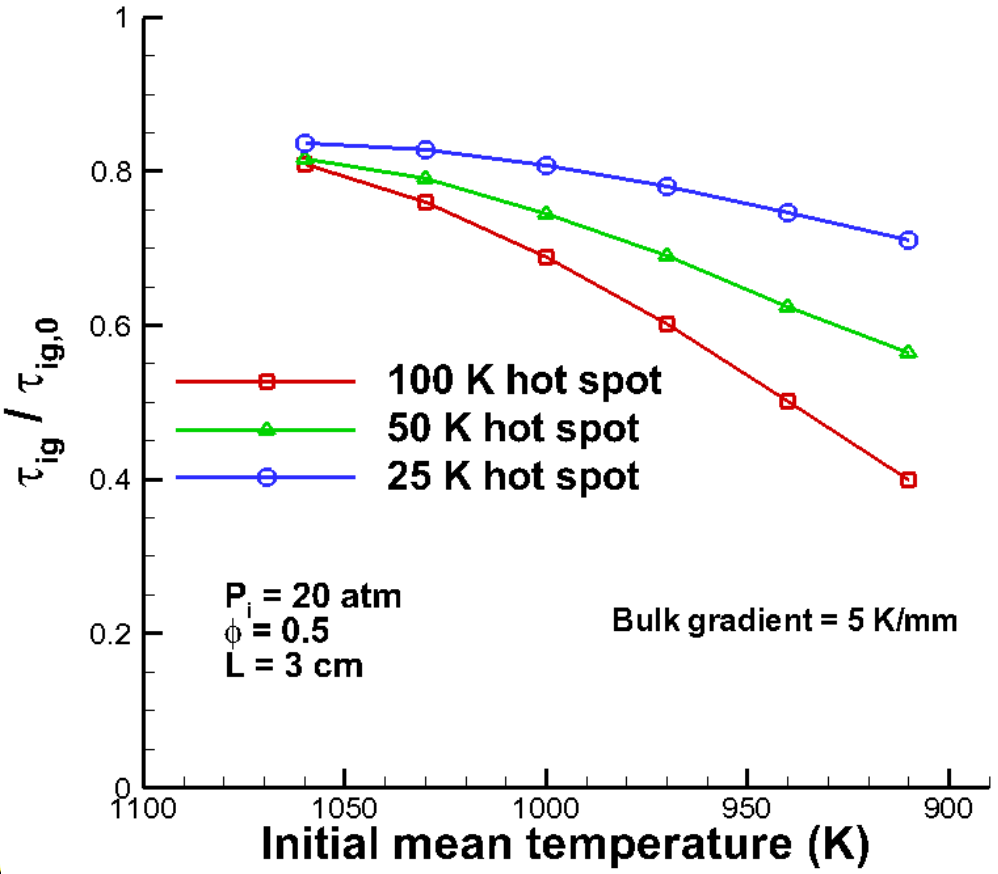


Constant mean T = 910 K

Hot Spot Autoignition (3)

King Abdullah University of Science and Technology KAUST

Parametric tests



$$\tau_{ig} \text{ determined at } \left.\frac{dP}{dt}\right|_{\max}$$

As the initial mean temperature is lowered, the net ignition delay becomes more sensitive to the level of temperature fluctuations.

Ignition Regime Criteria

King Abdullah University of Science and Technology KAUST

Turbulent Sankaran Number:

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

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

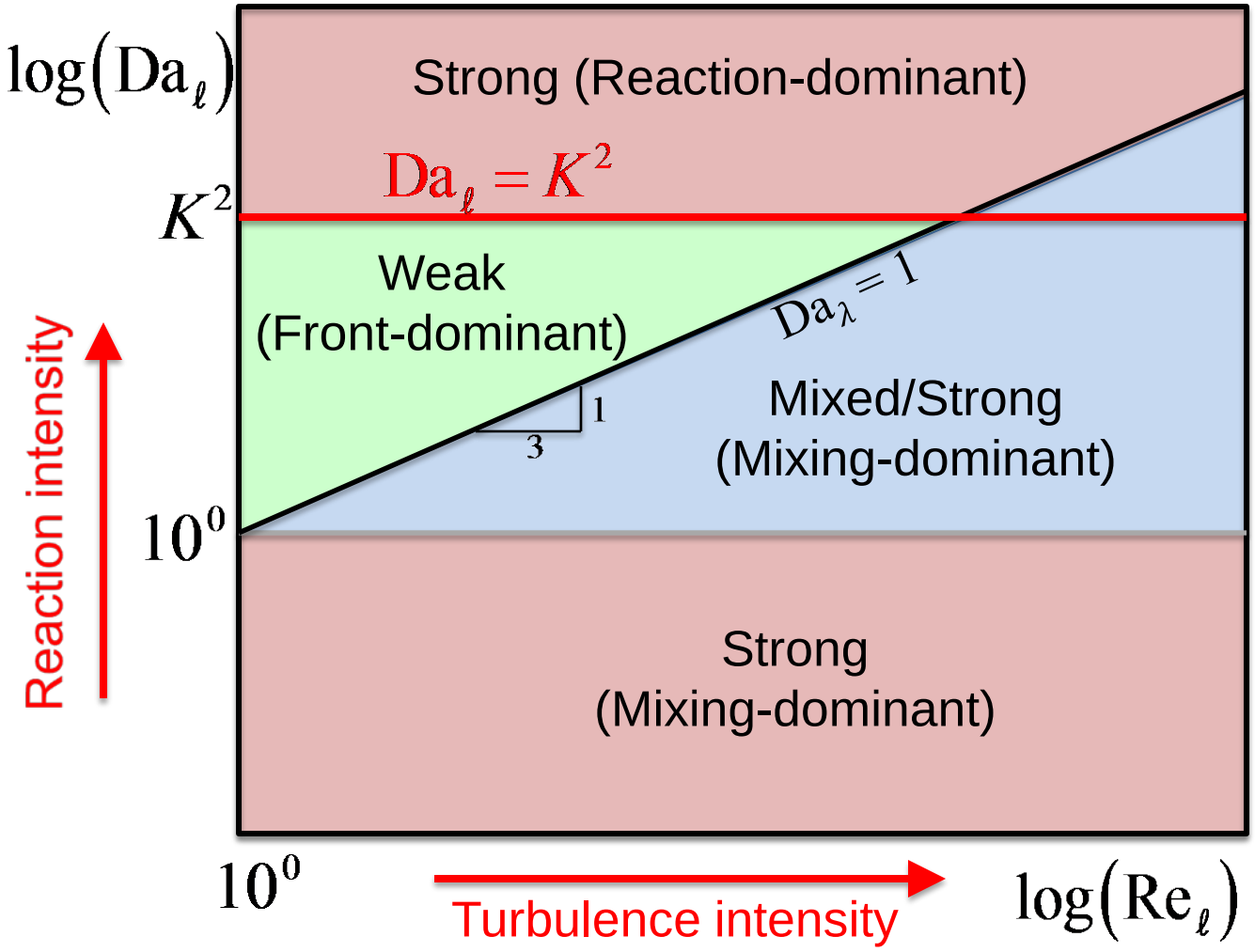
Ignition Criterion:
$$\begin{cases} \mathrm{Da}_\ell < K^2 & \text{Weak} \\ \mathrm{Da}_\ell > K^2 & \text{Strong} \end{cases}$$

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

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

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

The Regime Diagram



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

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

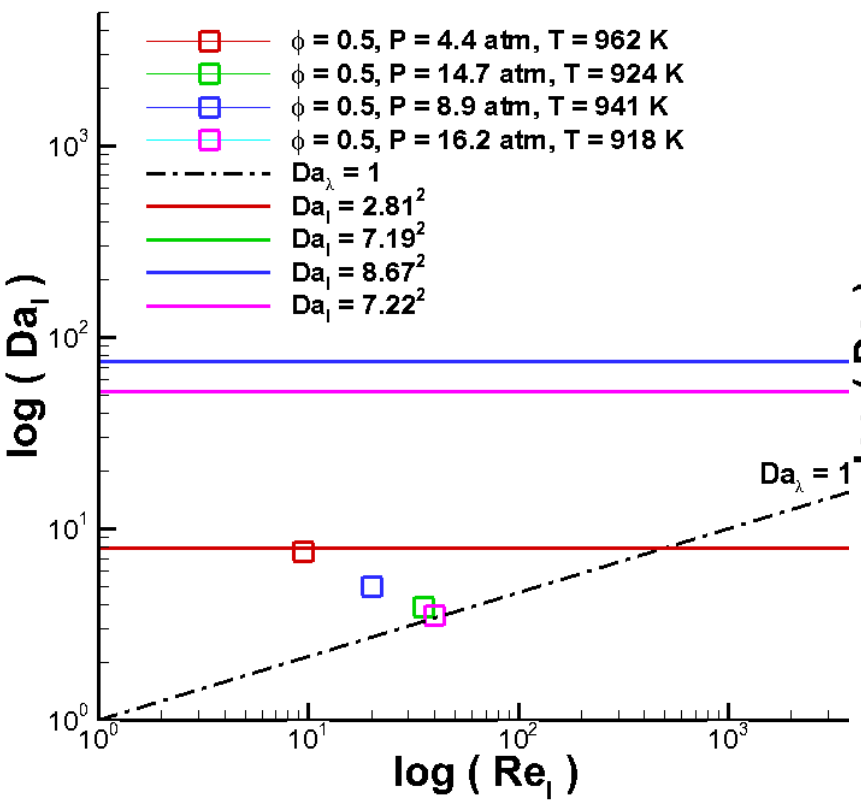
$$K = \beta \left(\frac{T'}{\tau_f} \right) \left(\frac{d\tau_{\mathrm{ig}}}{dT} \right)$$

Experimental Data on the Diagram

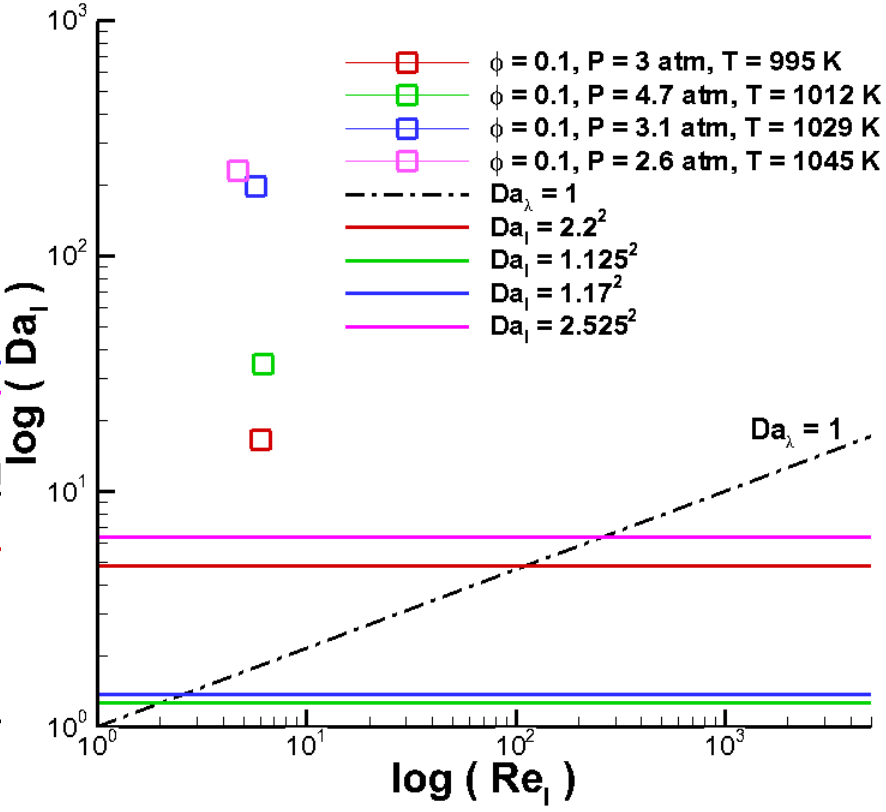
King Abdullah University of Science and Technology KAUST

Data from Mansfield & Wooldridge (2014)

Weak Ignition Cases



Strong Ignition Cases



Remarks & Work in Progress

King Abdullah University of Science and Technology KAUST

- The Sankaran-Zeldovich criterion combines both thermochemical property (*K*) of the mixture and the flow/scalar field conditions (Da_ℓ, Re_ℓ).

- 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.

- 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).

Work in Progress

- Multi-dimensional simulations (DNS) to demonstrate and validate the theory
- Extension of the ignition characterization for composition inhomogeneities
- Ignition characteristics for syngas at different composition/other fuels

Remarks & Future Work

King Abdullah University of Science and Technology KAUST

- A 1D numerical study incorporating detailed chemistry and transport is conducted over a mean temperature sweep of 850-1100 K at different compositions and pressures relevant to gas turbine operation to study the effect of thermal inhomogeneities on syngas ignition behavior.
- As the initial mean temperature is reduced, the ignition front behavior shifts from the spontaneous (strong) to deflagrative (weak) mode in the presence of a bulk thermal gradient.
- A non-dimensional parameter called the “Sankaran number” is shown to successfully capture the transition from strong to weak ignition.
- At sufficiently low temperatures however, passive scalar mixing tends to have a more pronounced effect on ignition characteristics as the mixing time scale becomes lower than the ignition time scale, thereby causing a transition of ignition behavior back to the spontaneous propagation mode.
- In the presence of thermal hot spots, enhanced compression heating of the end gas by the propagating front causes weak ignition behavior and faster thermal runaway at relatively lower temperatures. The trends are well captured by the Sa.

- Future work (work in progress):
  - Multi-dimensional DNS to study statistical effects of turbulence
  - Extend the Sankaran criterion in turbulent conditions