Prediction of auto-ignition regimes in turbulent reacting flows with thermal inhomogeneities

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Introduction

Both strong (homogeneous) and weak (inhomogeneous) ignition regimes have been observed in experimental studies [1]. Occurrence of weak ignition was found to result in significant advancement of ignition delay. The strong ignition limit was well predicted in laminar flows by the a priori *Sankaran criterion* [2].

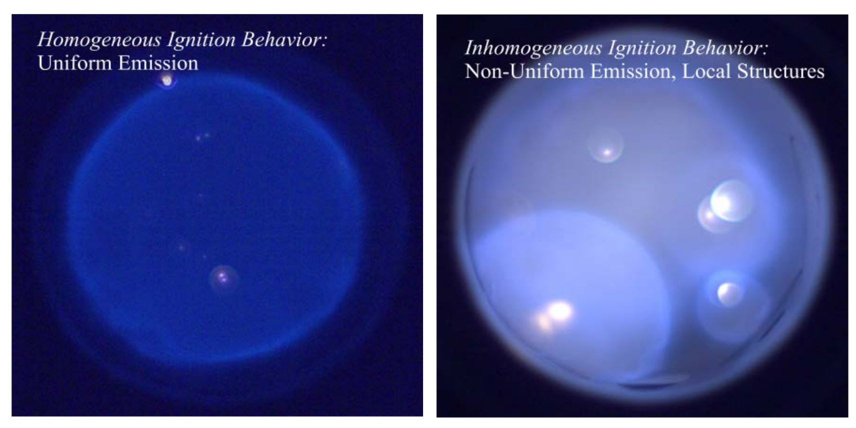
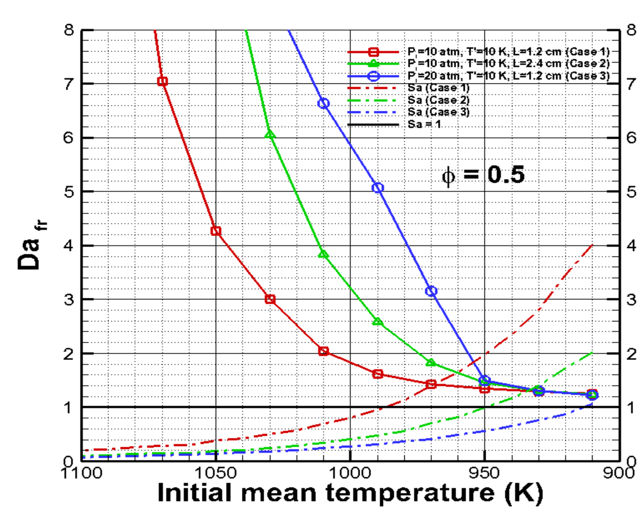


Figure 1: Strong and weak ignition regimes [1]



$$\beta \frac{S_L}{S_{sp}} < 1$$

$$\beta S_L \frac{dT}{dx}\left|\frac{d\tau_{ig}}{dT}\right| < 1$$

Figure 2: Front Damkohler and Sankaran numbers versus mean temperature for syngas-air mixture [2]

❑ **Objective:** To extend the Sankaran criterion to account for the effects of turbulent fluctuations and validate the turbulent ignition criteria.

Turbulent Ignition Regime Prediction

❑ Sankaran criterion

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

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

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

$$\mathrm{Sa} = K\mathrm{Da}_\ell^{-1/2} \qquad K = \beta\left(\frac{T'}{\sqrt{\tau_{ig}\tau_f}}\right)\left(\frac{d\tau_{ig}}{dT}\right)$$

$$\mathrm{Da}_\ell = \frac{\tau_\ell}{\tau_{ig}}$$ Integral Damkohler number

Ignition criterion ➡ $\begin{cases} \mathrm{Da}_\ell < K^2 & \text{weak} \\ \mathrm{Da}_\ell > K^2 & \text{strong (reaction-dominant)} \end{cases}$

❑ Mixing criteria

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

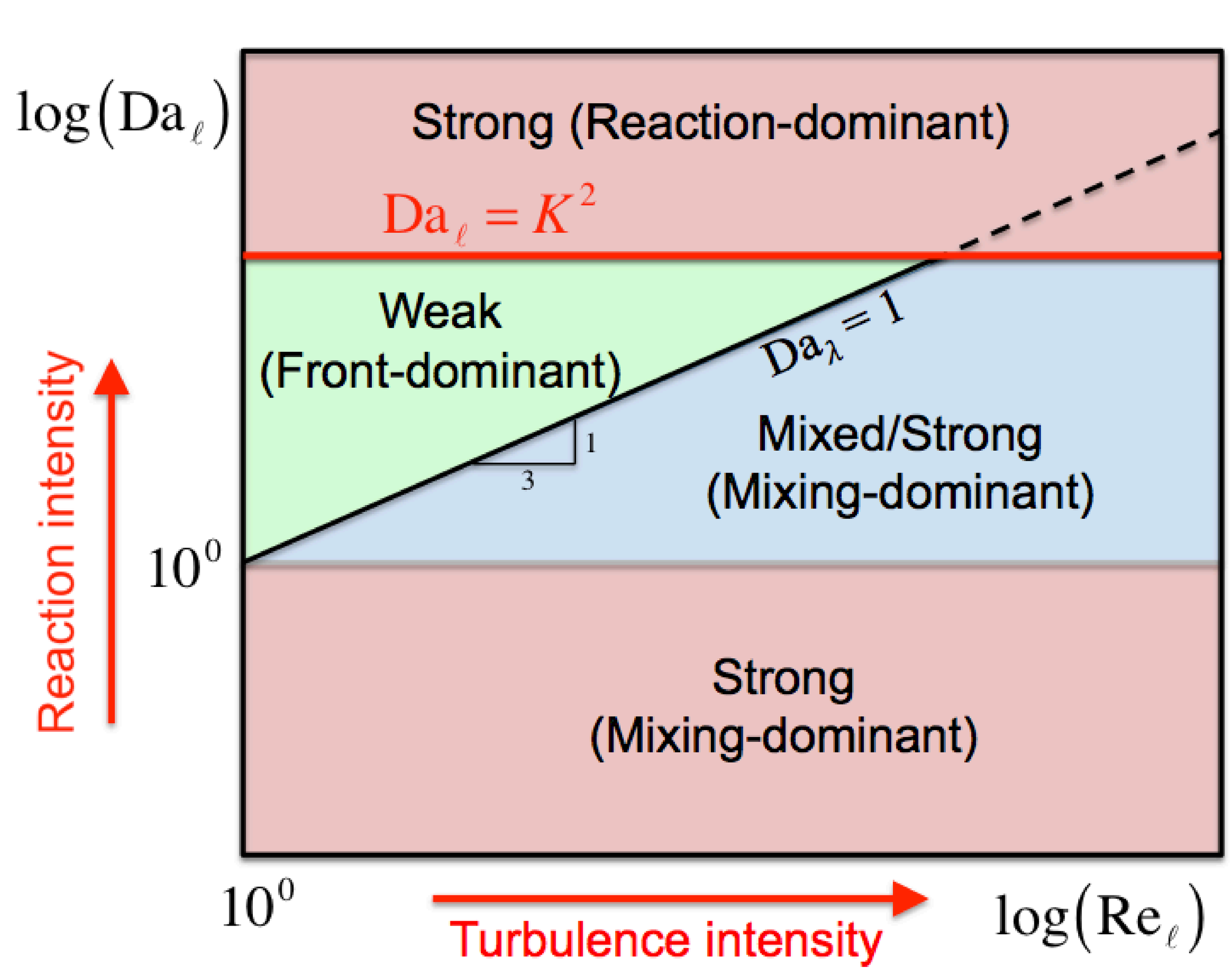
$$\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{ig}} = \frac{\tau_\lambda}{\tau_{ig}} = \frac{\tau_\ell}{\tau_{ig}}\frac{\tau_\lambda}{\tau_\ell} = \mathrm{Da}_\ell \mathrm{Re}_\ell^{-1/3}$$

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

$$\mathrm{Da}_\lambda = \mathrm{Da}_\ell \mathrm{Re}_\ell^{-1/3} \begin{cases} \mathrm{Da}_\lambda > 1 & \rightarrow \text{weak} \\ \mathrm{Da}_\lambda < 1 & \rightarrow \text{Mixed/strong (mixing-dominant)} \end{cases}$$

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

Turbulent Ignition Regime Diagram



Ignition regime criteria

$$\begin{cases} \mathrm{Da}_\ell > K^2: & \text{Reaction-dominant strong ignition} \\ 1 < \mathrm{Da}_\ell < K^2, \mathrm{Da}_\lambda > 1: & \text{Weak ignition} \\ \mathrm{Da}_\lambda < 1, \mathrm{Da}_\ell > 1: & \text{Mixing-dominant mixed/strong ignition} \\ \mathrm{Da}_\ell < 1: & \text{Mixing-dominant strong ignition} \end{cases}$$

Regime Diagram Validation: DNS Study

Table 1: 2D syngas/air DNS parametric cases: P_0 = 20 atm, φ = 0.5, H_2: CO = 0.7:1 (molar)

Case	T_0 (K)	τ_{ig} (ms)	T' (K)	K^2	ℓ (mm)	u' (m/s)	τ_ℓ (ms)	Da_ℓ	Re_ℓ	Da_λ	τ_{HRR_max}/τ_{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 kinetic energy spectrum employed.
- Uncorrelated temperature and velocity fields.
- Hot spot superimposed on the random T field at the center of the domain.
- Detailed chemical kinetic mechanism for syngas with 12 species and 33 reactions.

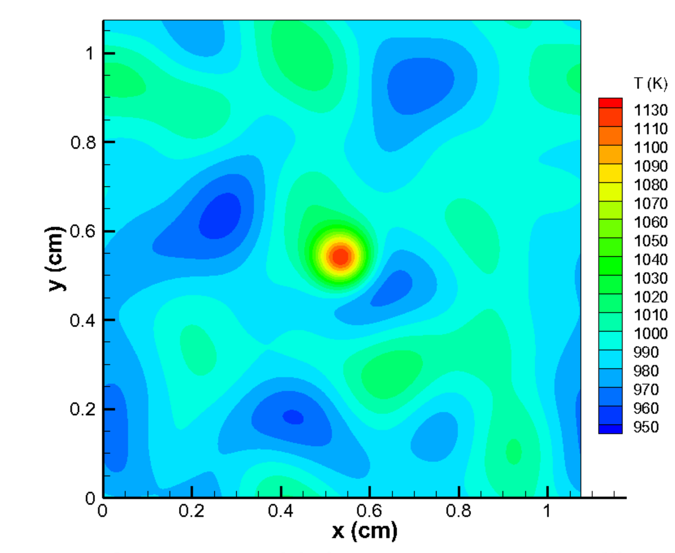


Figure 3: Initial temperature profile (case A)

Results and Discussion

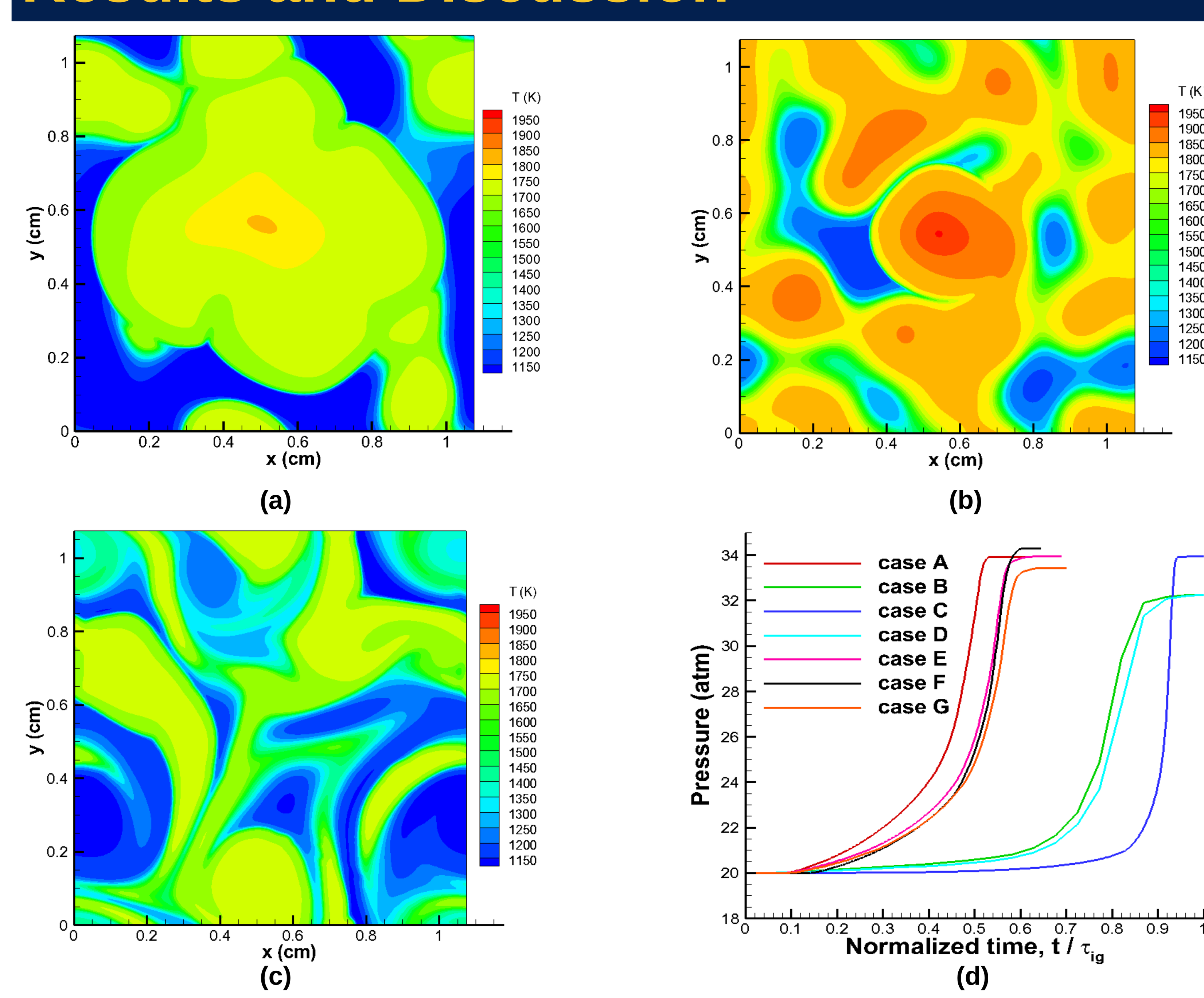


Figure 4: Temperature fields at 50% heat release rate: (a) case A (weak), (b) case B (reaction-controlled strong) and (c) case C (mixing-controlled strong), (d) pressure traces for all cases. Case A ignites much earlier due to enhanced compression heating effect of the propagating deflagrative fronts, whereas cases B and C show no appreciable flame propagation and auto-ignite nearly homogeneously at nearly the corresponding homogeneous ignition delay timings.

Conclusions

❑ In the present work, a non-dimensional scaling analysis is performed based on the homogeneous theory of turbulence to derive various criteria to predict strong and weak ignition regimes.
❑ The ignition regime criteria are further validated against 2D direct numerical simulations (DNS) of auto-ignition of a lean syngas-air mixture.

Acknowledgements

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References

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❑ P. Pal, A. Mansfield, P.G. Arias, M. Wooldridge, H.G. Im, *Combust. Theory. Modell.* 19 (2015) 587-601.