Evaluation of Hydrogen, Propane and Methane-Air Detonations Instability and Detonability

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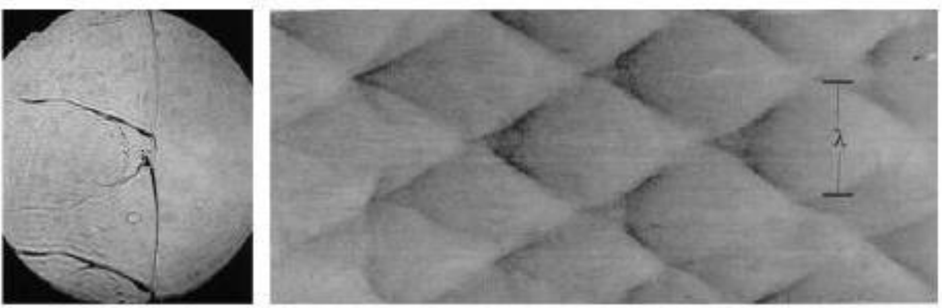
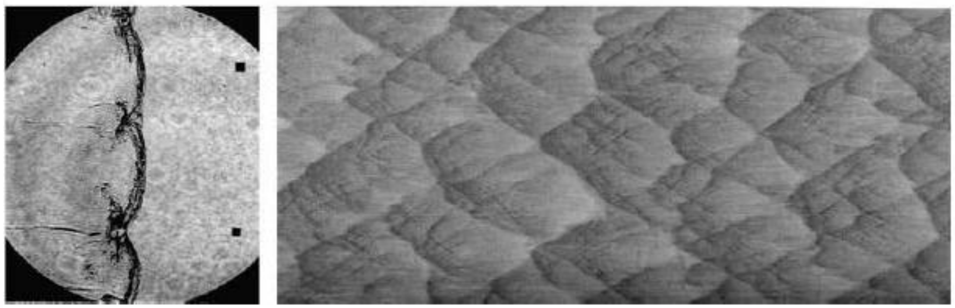
Detonability

- ✓ Conventionally assessed by the ignition delay or alternatively the cell size.
- ✓ Draw Back : Differentiating between mixtures known to behave differently :
  - ✓ Mixtures with irregular structure found to be more detonable [Moen et al. 1986], [Desbordes et al. 1993], [Desbordes 1988], [Kuznetsov et al. 2000], [Radulescu & Lee 2002] and [Radulescu 2003]

Irregularity and The detonability

- [Shepherd 2009]





$2H_2 + O_2 + 17\,Ar$

$C_3H_8 + 5O_2 + 9\,N_2$

Characteristic stability Parameter

A Parameter to correlate with Detonability

$$\chi = \frac{t_i}{t_e}\frac{E_a}{RT}\frac{Q}{RT}$$

$$a_c = \frac{c\chi}{t_i} = \frac{c}{t_e}\frac{E_a}{RT}\frac{Q}{RT}$$

[Short & Sharpe 2003], [Radulescu 2003], [Ng et al. 2005], [Bradley 2012], [Tang & Radulescu 2013]

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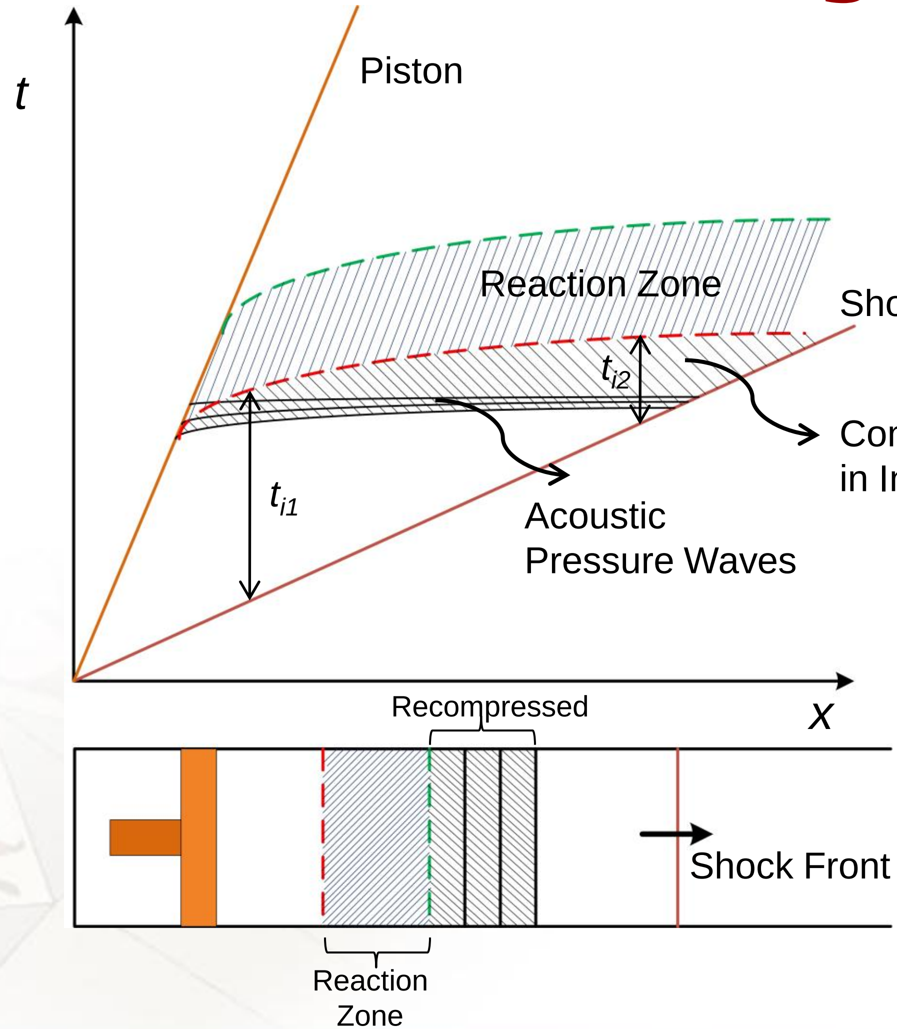
Piston Induced Shock Ignition



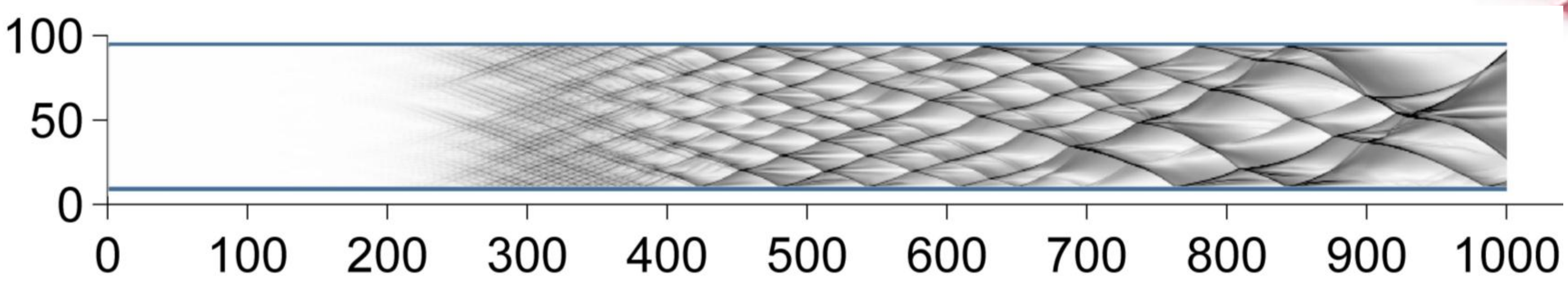
$$\chi = \frac{t_i}{t_e}\frac{E_a}{RT}\frac{Q}{RT}$$

[Sharpe 2003 , Tang & Radulescu 2013]

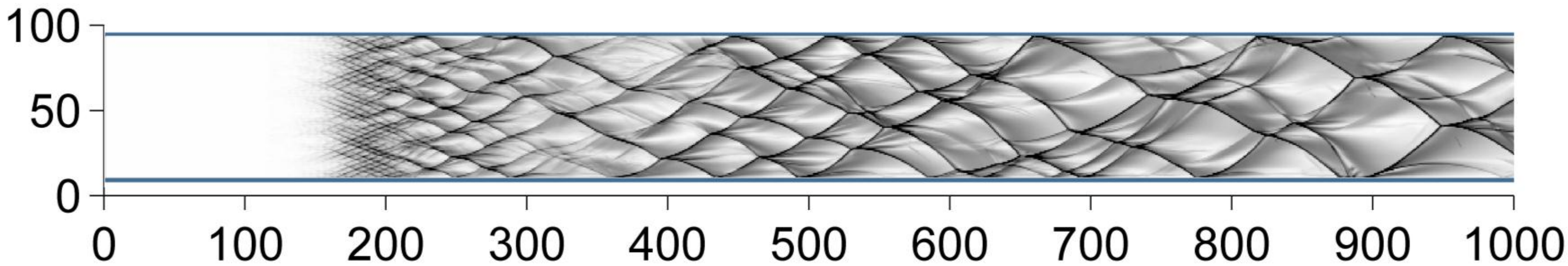
Instability Growth Rates

- ✓ Short & Sharpe 2003, Ng et al 2005 and Leung et al 2010, investigated Influence of χ on the stability of 1D detonations
- ✓ Critical χ value of 50-100 for the onset of instabilities

Instability Growth Rates



Numerical soot foil for a mixture with χ=24



Numerical soot foil for a mixture with χ=95

[Borzou et al. 2011]

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Goals

Measuring the value of characteristic χ parameter in fuel-air mixtures at atmospheric conditions.

Observing the influence of χ on cellular dynamics of detonations in those mixtures.

Stability Parameter Calculations

Performed for:

- ✓ A range of compositions from the lean to the rich limit for a variety of hydrogen, methane and propane-air mixtures.
- ✓ By extraction of (t_i), (t_e), (E_a) and (Q).
- ✓ Numerous ways to extract meaningful values [Browne et al. 2004], [Liang et al. 2007] and [Radulescu 2003]

Ignition Delay

✓Post-shock VN state calculated with NASA CEA code [1]

✓Kinetic properties of VN state obtained with constant volume ignition calculations: Cantera Package [2]

✓Detailed Kinetic Models:

- Li et al. [3] for hydrogen mixture
- Sandiego [4] for propane mixture
- GRI 3.0 [5] for methane mixture

[1] McBride, B.J., Gordon, S., Technical Report E-8017-1, National Aeronautics and Space Administration, Washington D.C., June 1996

[2] Goodwin D., Caltech, Pasadena, 2009.

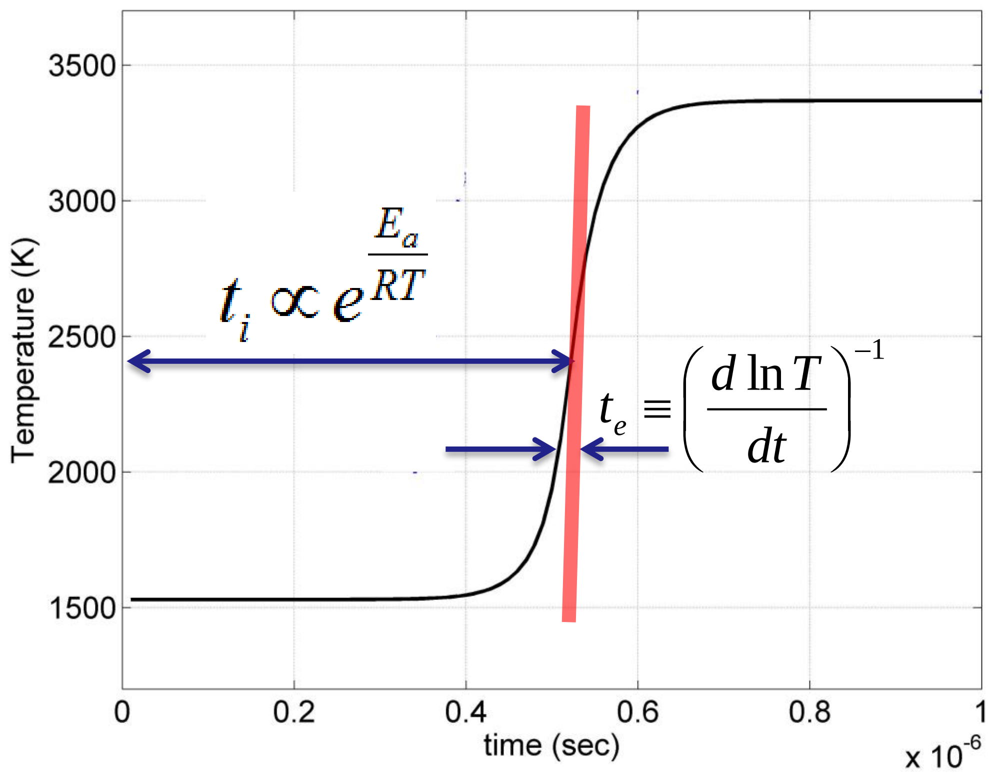
[3] J. Li, Z. Zhao, A. Kazakov, and F. L. Dryer, International Journal of Chemical Kinetics, (2004)

[4] http://combustion.ucsd.edu, University of California at San Diego.

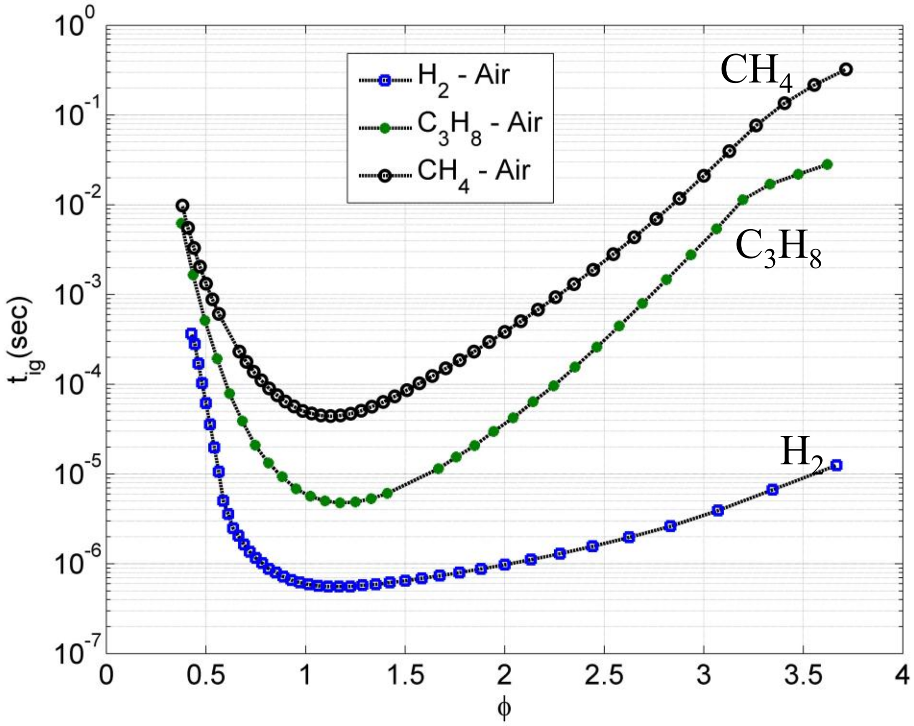
[5] http://www.me.berkeley.edu/gri_mech/

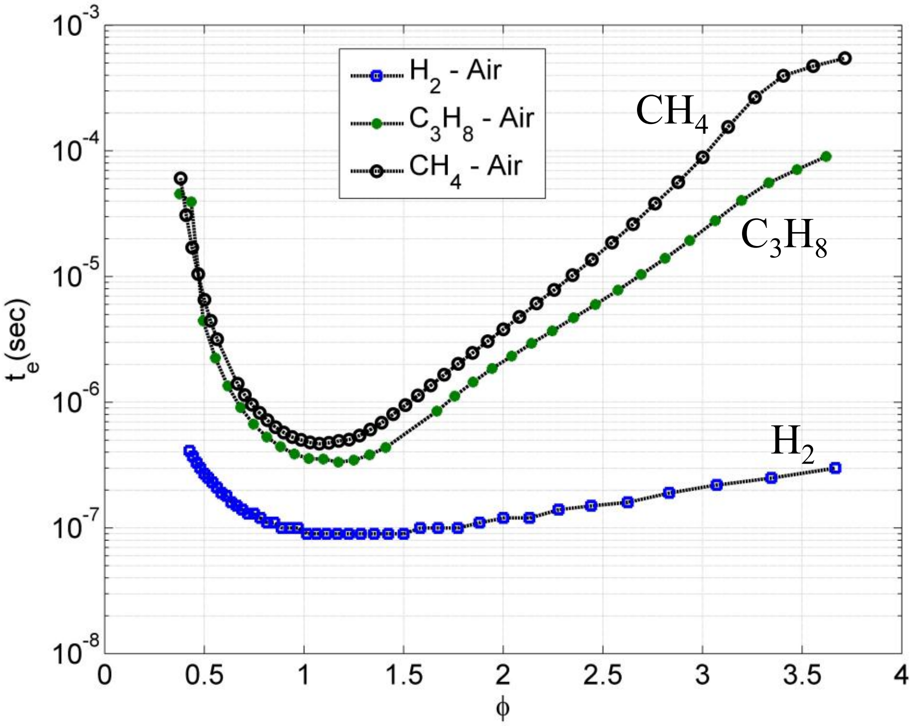
Ignition Delay

An example of calculations for H_2-Air stoichiometric

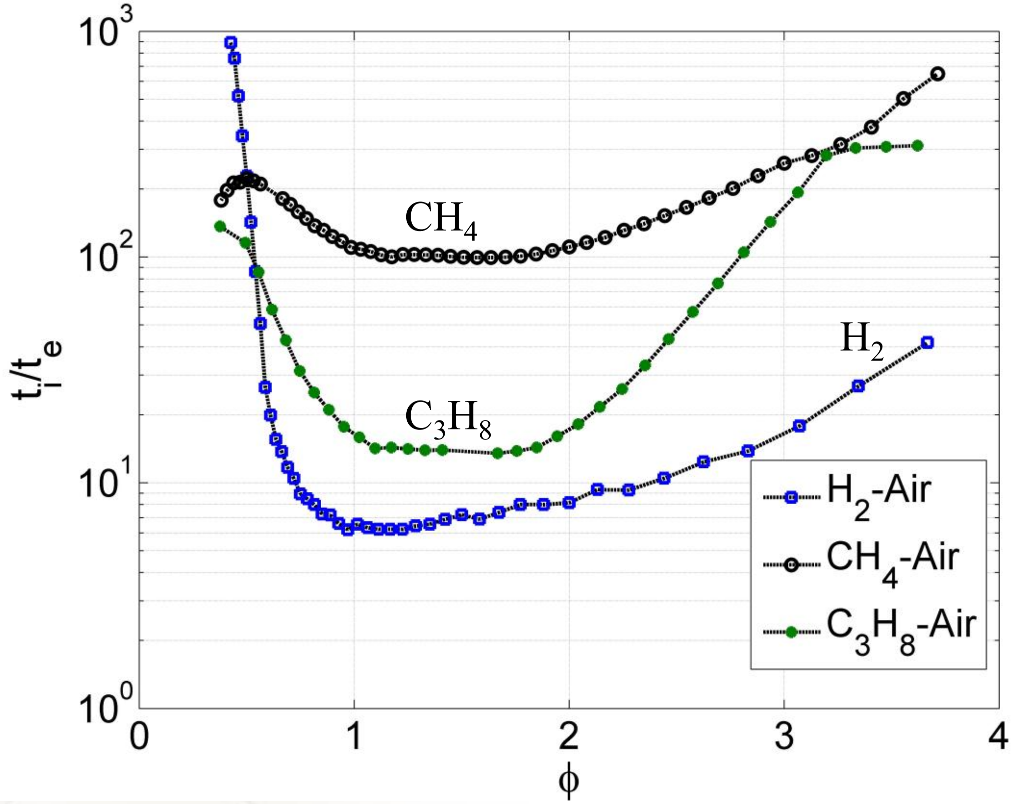


Ignition Delay & Reaction Time

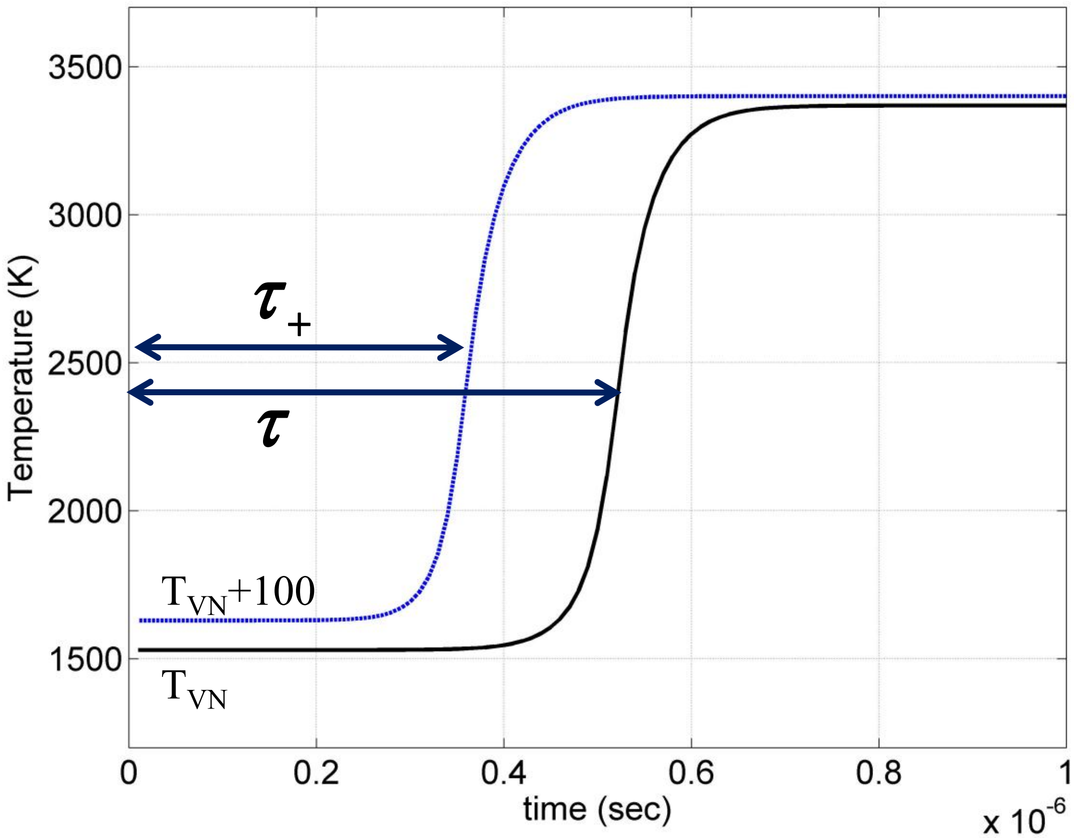




Induction to Reaction Time Ratio



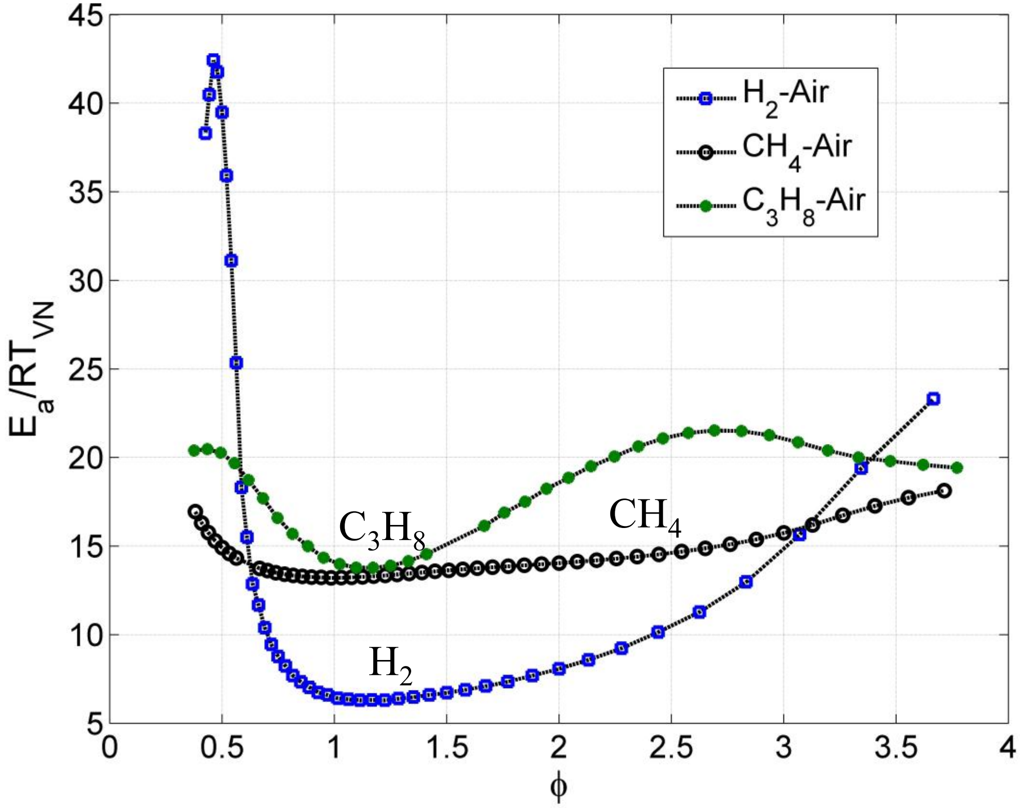
Activation Energy



$$t_i \propto exp\left(\frac{E_a}{RT}\right)$$

$$\frac{E_a}{RT_{vN}} = \frac{1}{T_{vN}}\left(\frac{\ln(\tau_+)-\ln(\tau)}{1/T_{vN+} - 1/T_{vN}}\right)$$

Activation Energy



Heat Release

- M_{CJ} and γ_{VN} obtained by calculations in NASA CEA code.
- Heat release extracted from equilibrium calculations using perfect gas model.

$$\frac{Q}{RT_0} = \frac{\gamma}{2\left(\gamma^2 - 1\right)}\left(M_{CJ} - \frac{1}{M_{CJ}}\right)^2$$

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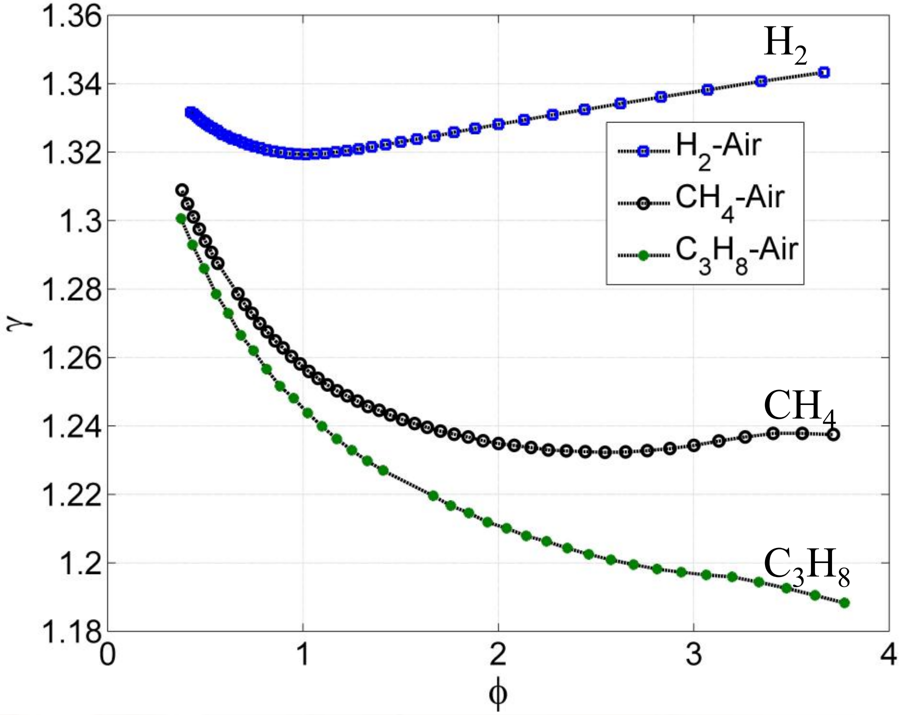
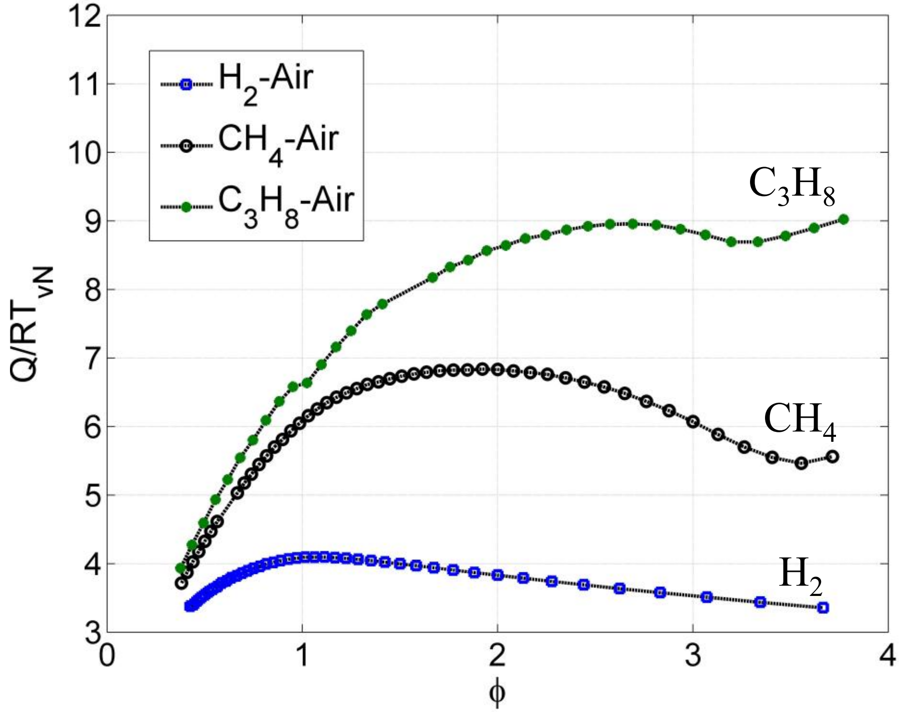
Heat Release & Isentropic Heat Ratio





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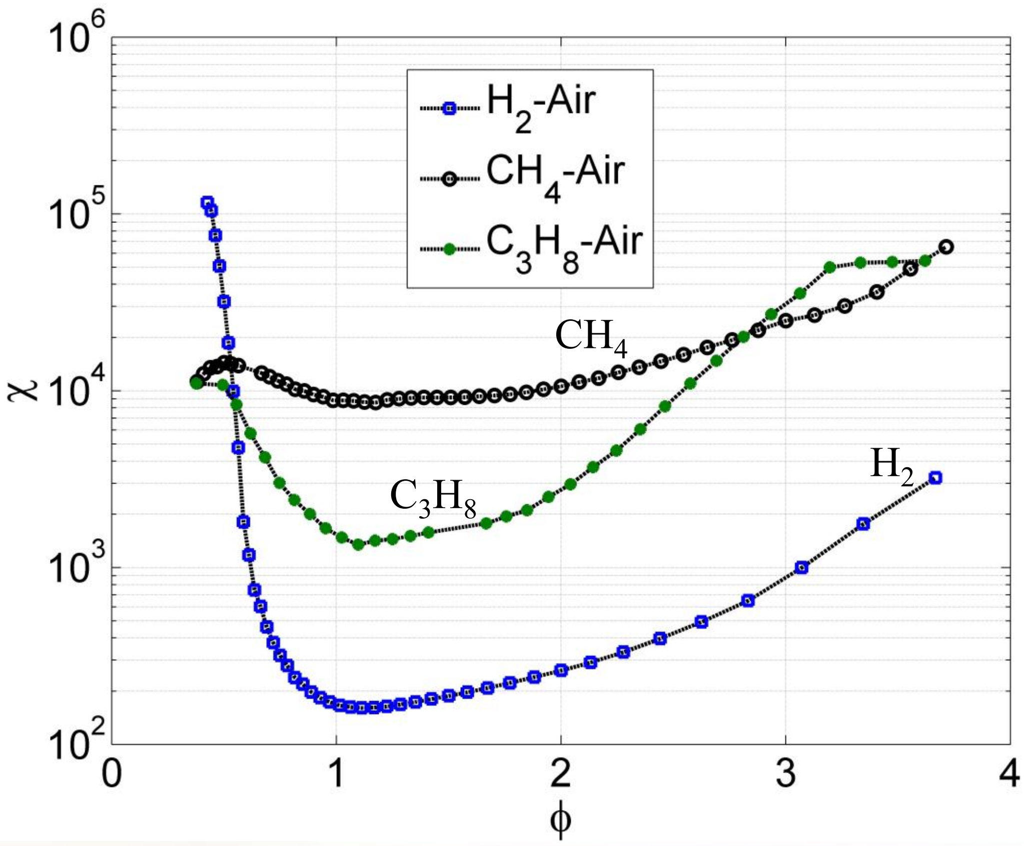
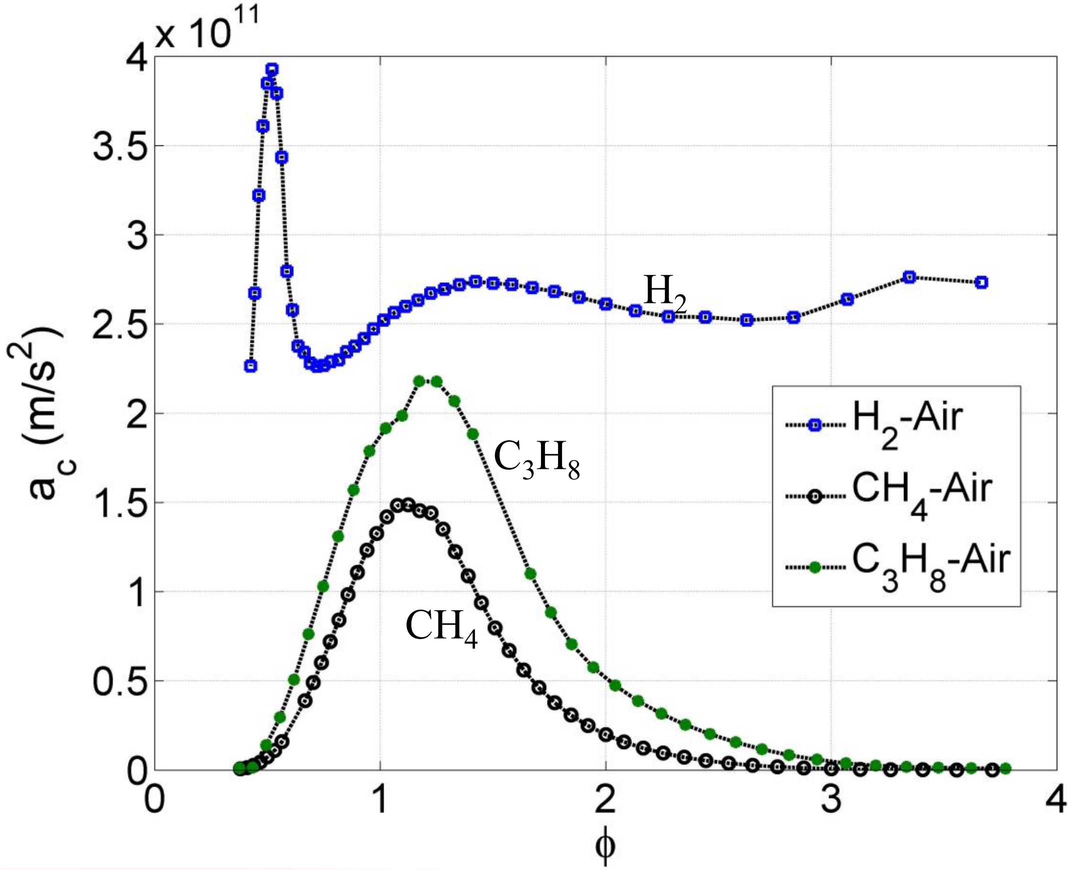
Characteristic Stability Parameter



Reaction Zone Acceleration



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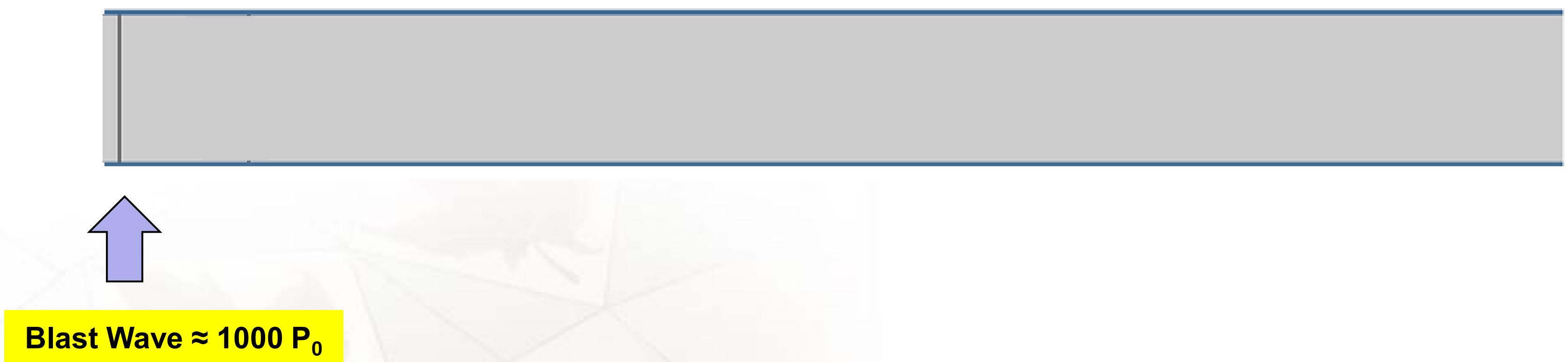
Modeling

Performing numerical simulations for :

- ✓ Further studying the link between cellular instability and the χ parameter.
- ✓ Focusing on the stability of overdriven detonation waves in a reactive gas.
- ✓ Planar blast waves originating from a plane source of energy, which decay towards self-sustained detonations.
- ✓ Monitoring the onset of instabilities on the structure of the reactive blast wave during the shock decay.

Modeling

✓ Stoichiometric H_2, C_3H_8 and CH_4 air mixtures with the corresponding χ parameter values of 132, 1920 and 7260 respectively.



Modeling

- Solving the reactive Euler equations coupled with the two step model using the AMRITA (J.J. Quirk) computational facility

$$\frac{D\rho}{Dt} + \rho \nabla . U = 0 \qquad \frac{DU}{Dt} + \frac{1}{\rho}\nabla P = 0 \qquad \frac{D}{Dt}(e + \lambda_r Q) + P\frac{D}{Dt}\left(\frac{1}{\rho}\right) = 0$$

- Where, for an ideal gas

$$e = \frac{1}{\gamma - 1}\frac{P}{\rho}$$

$$\begin{cases} \dfrac{D\lambda_i}{Dt} = -K_i H(\lambda_i)\exp\left(-\dfrac{E_a}{RT}\right) \\ \dfrac{D\lambda_r}{Dt} = \left(1 - H(\lambda_i)\right)K_r(1-\lambda_r)^{\upsilon} \end{cases}$$

128 GPI Resolution

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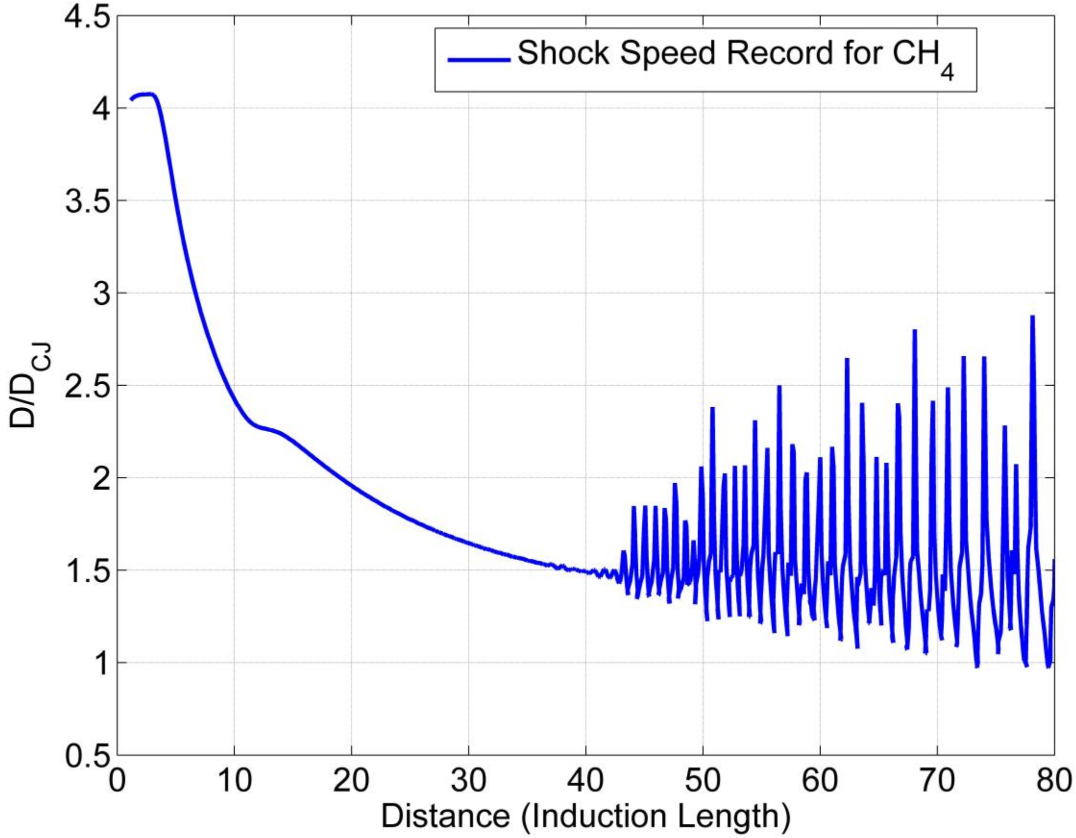
Instability Growth



CH_4-Air χ=7260

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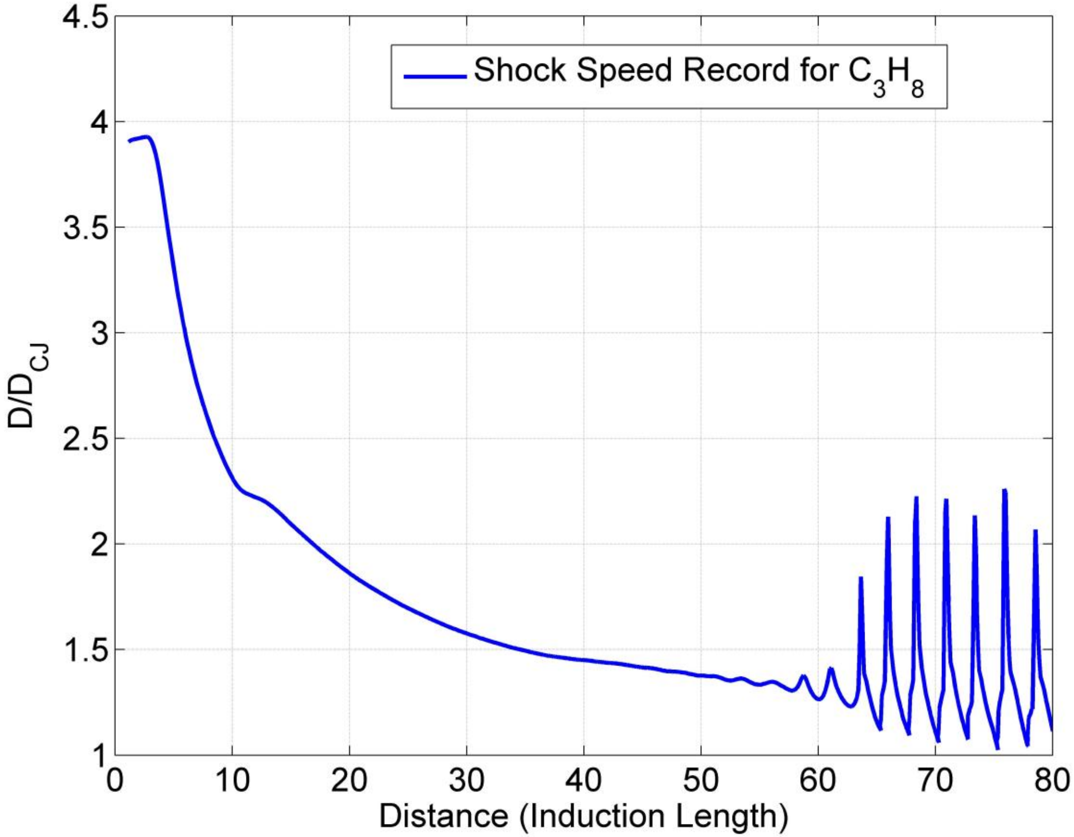
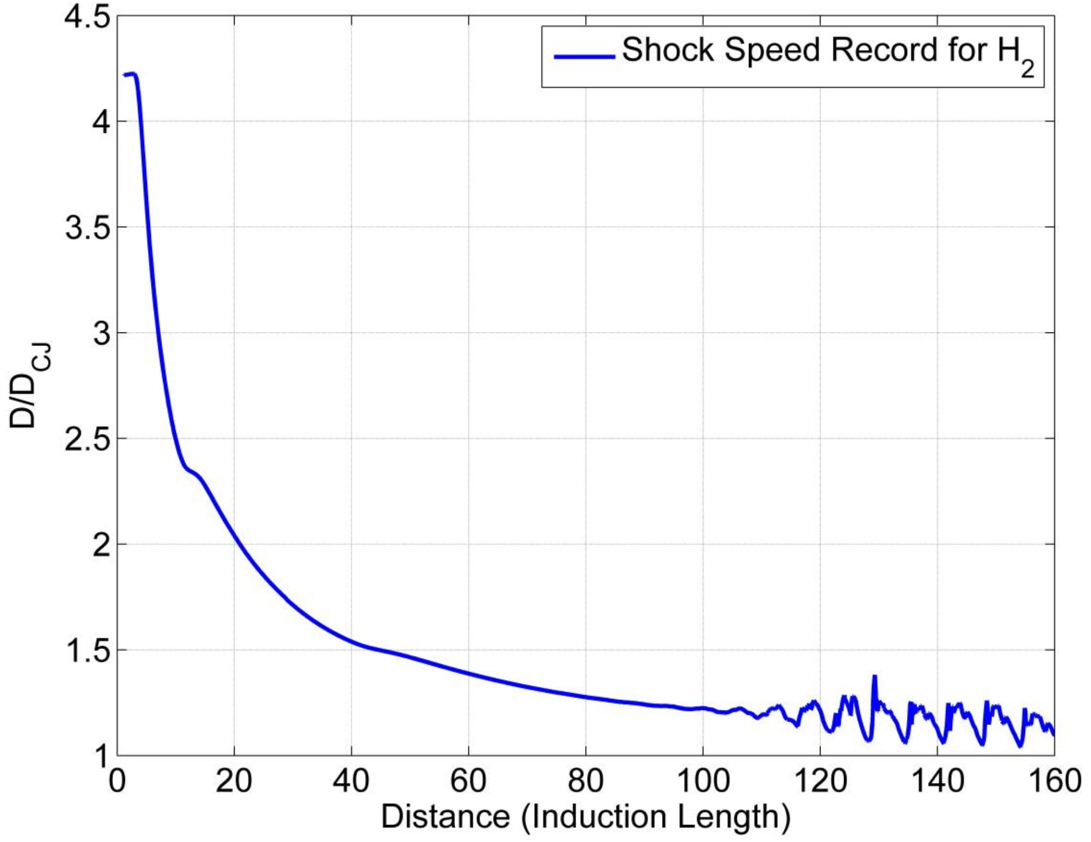
Instability Growth



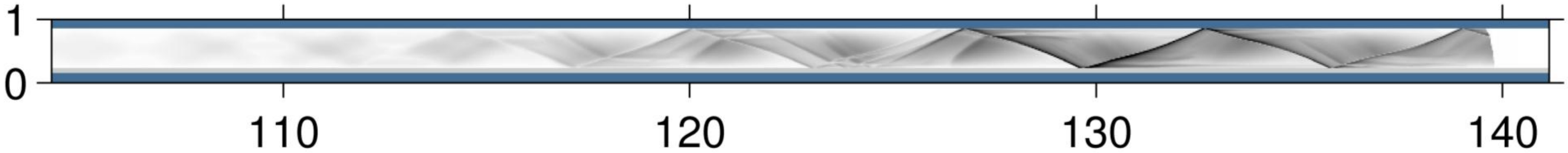
C_3H_8-Air χ =1920

Instability Growth



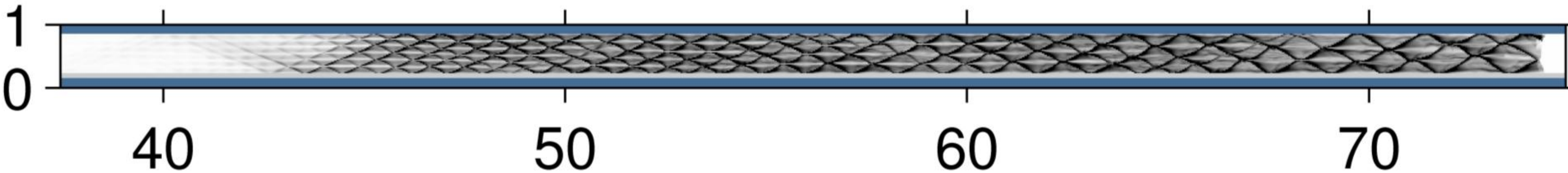
H_2-Air χ =132

Instability Growth



H_2-Air χ =132

C_3H_8-Air χ =1920



CH_4-Air χ =7260

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Concluding Remarks

- ✓ Characteristic χ parameter was evaluated for fuel-air mixtures at atmospheric conditions.
  - ✓ Methane was found much more unstable than others with the highest values of χ parameter.

$$\chi_{CH_4} >> \chi_{C_3H_8} >> \chi_{H_2}$$

- ✓ Simulations showed that a methane-air mixture develops cellular structures more readily than propane and hydrogen, when observed on similar induction time scales.

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