Explosive Mode Analysis for Computational Flame Diagnostics with Detailed Chemistry

Tianfeng Lu
University of Connecticut

Chung K. Law
Princeton University

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Background

- Governing equations for a discretized reacting flow

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}) = \boldsymbol{\omega}(\mathbf{y}) + \mathbf{s}(\mathbf{y})$$

y: vector of variables (e.g. T, **C**)
ω: chemical source term
s: mixing term

- The Jacobian $\mathbf{J} = \frac{\partial \mathbf{g}}{\partial \mathbf{y}} = \mathbf{J}_{\boldsymbol{\omega}} + \mathbf{J}_{\mathbf{s}}$, $\mathbf{J}_{\omega} = \frac{\partial \boldsymbol{\omega}}{\partial \mathbf{y}}$, $\mathbf{J}_{\mathbf{s}} = \frac{\partial \mathbf{s}}{\partial \mathbf{y}}$

- Jacobian analysis for combustion: e.g. ILDM (Maas & Pope); CSP (Lam); Explosive mode analysis with CSP (Fotache, et al; Kazakov et al)
- Explosive mode analysis at different levels
  - Full Jacobian ($\mathbf{J}_{\mathbf{g}}$)
    Explosive mode analysis (EMA): $\mathrm{Re}(\lambda(\mathbf{J}_{\mathbf{g}})) > 0$
  - Chemical Jacobian ($\mathbf{J}_{\boldsymbol{\omega}}$) for chemical properties (Lu, et al)
    Chemical explosive mode analysis (CEMA): $\mathrm{Re}(\lambda(\mathbf{J}_{\boldsymbol{\omega}})) > 0$

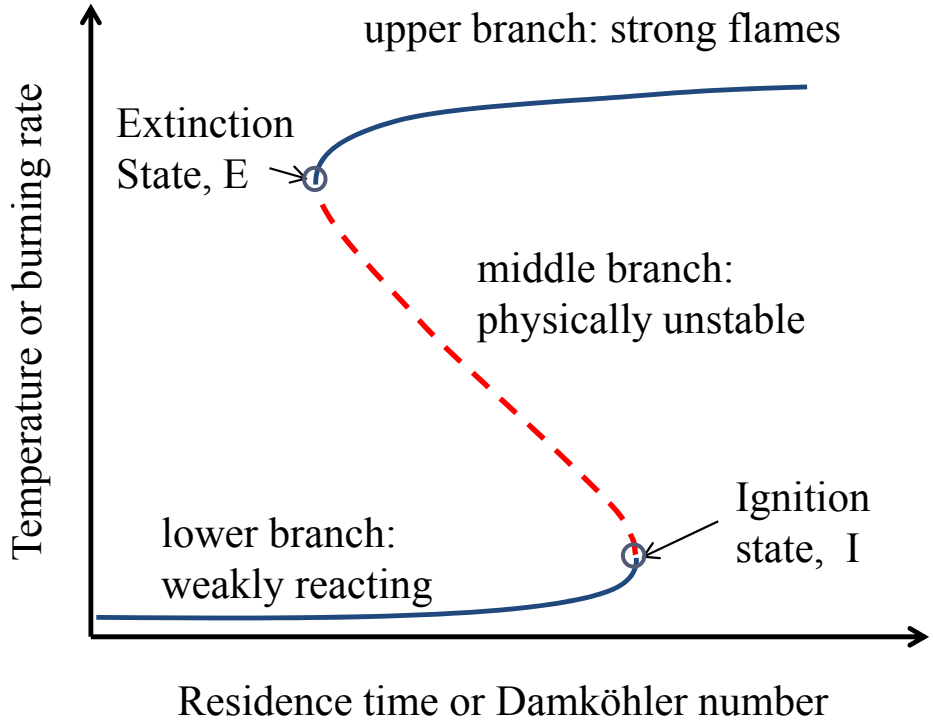
Part I.

Explosive Mode Analysis (**EMA**):

Flame Stability in Perfectly Stirred Reactors (PSR)

Background:
Stability of Steady State Flames

- The canonical "S"-curve



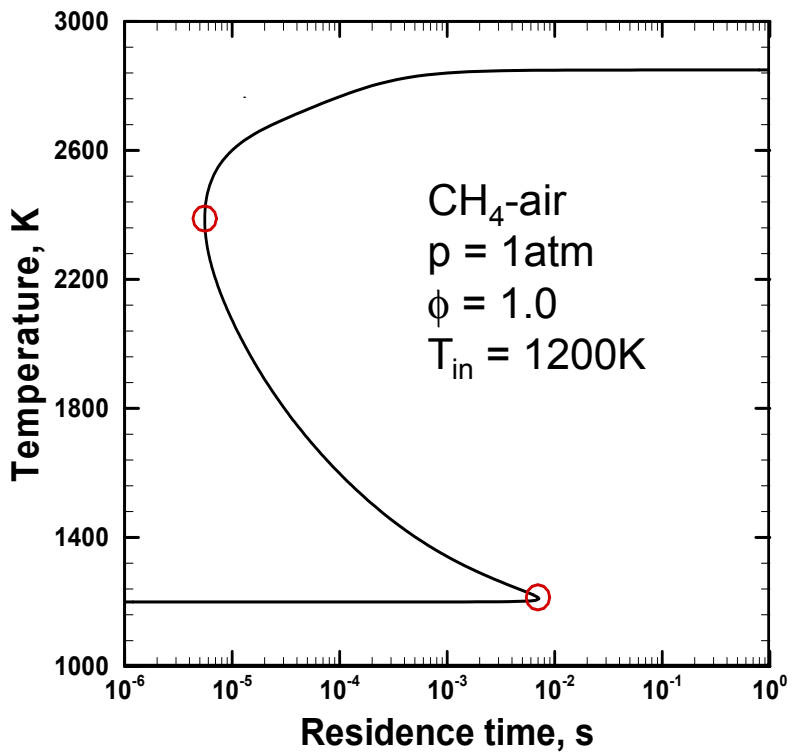
$\lambda_i(\mathbf{J_g}) = 0$ at turning points

J is the full Jacobian

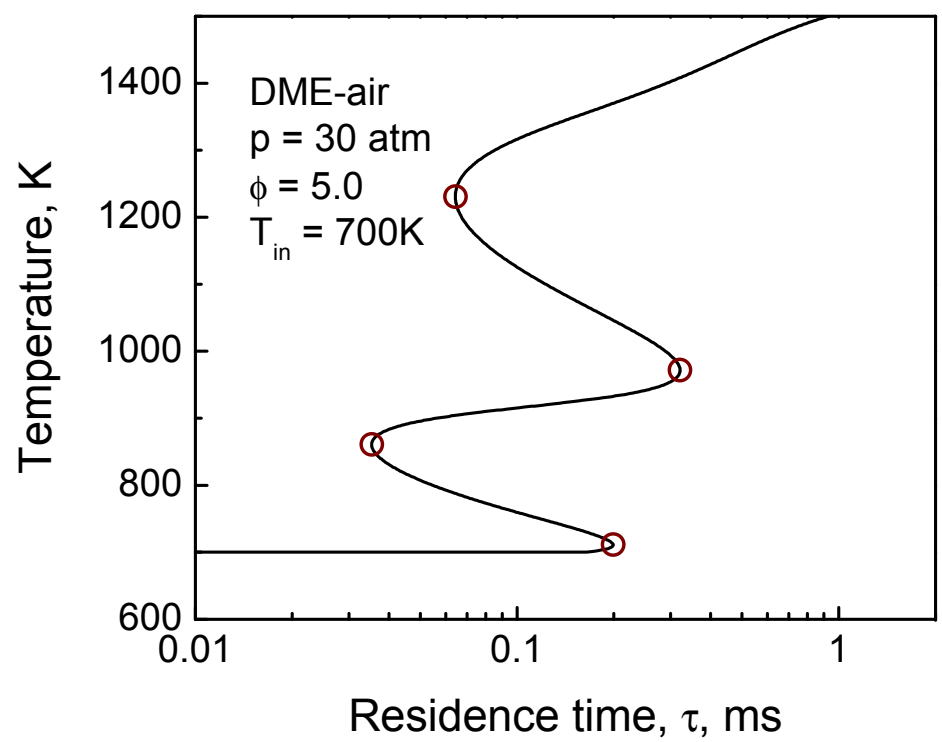
- Ignition/extinction limits are important for mechanism validation, e.g. with counterflow flames

"S"-Curves for Practical Fuels in PSR

CH_4-air, GRI3.0

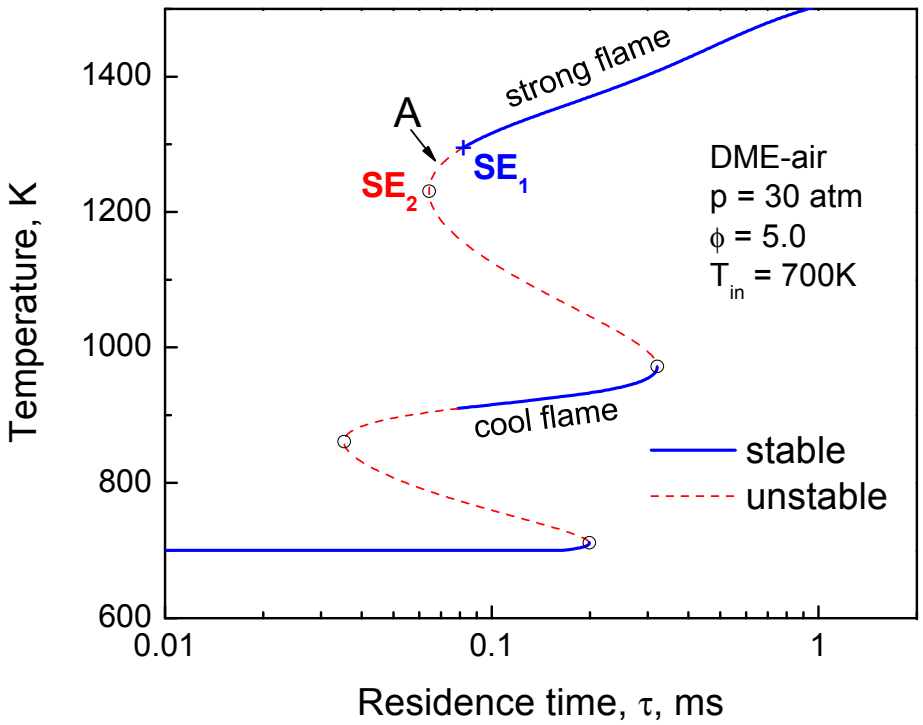


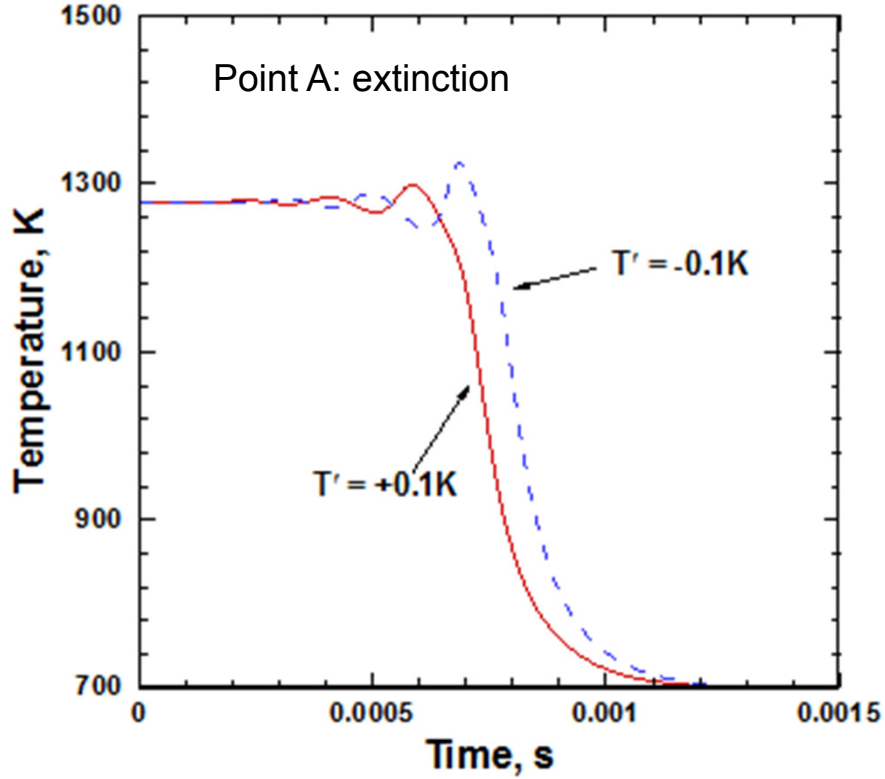
DME-air, with NTC



- Fuels with NTC feature multiple criticalities
- Are the turning points physical ignition/extinction states?

EMA for DME-air in PSR (1/3)

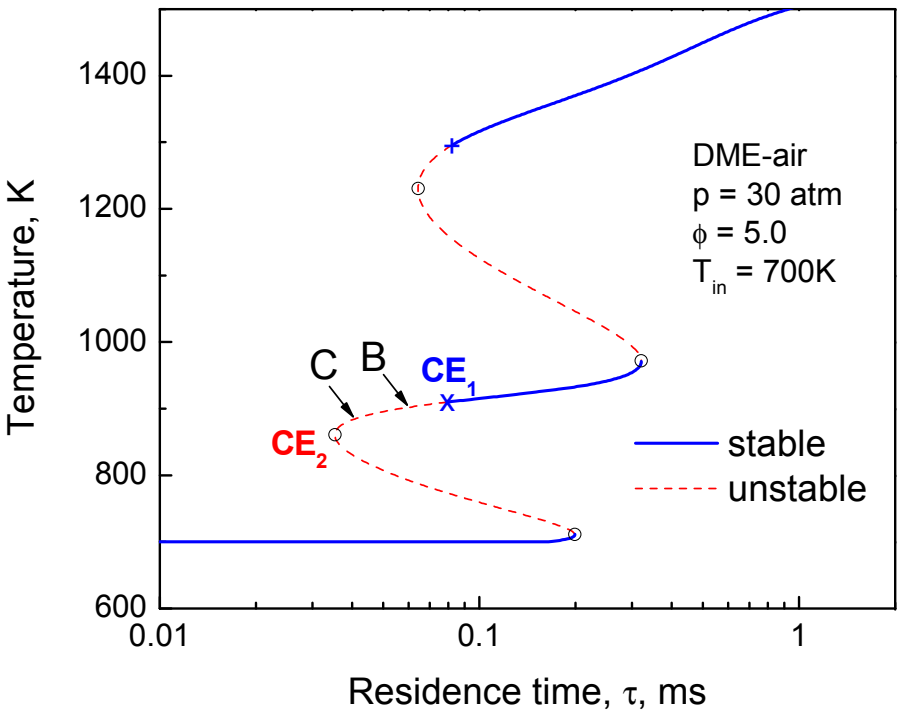


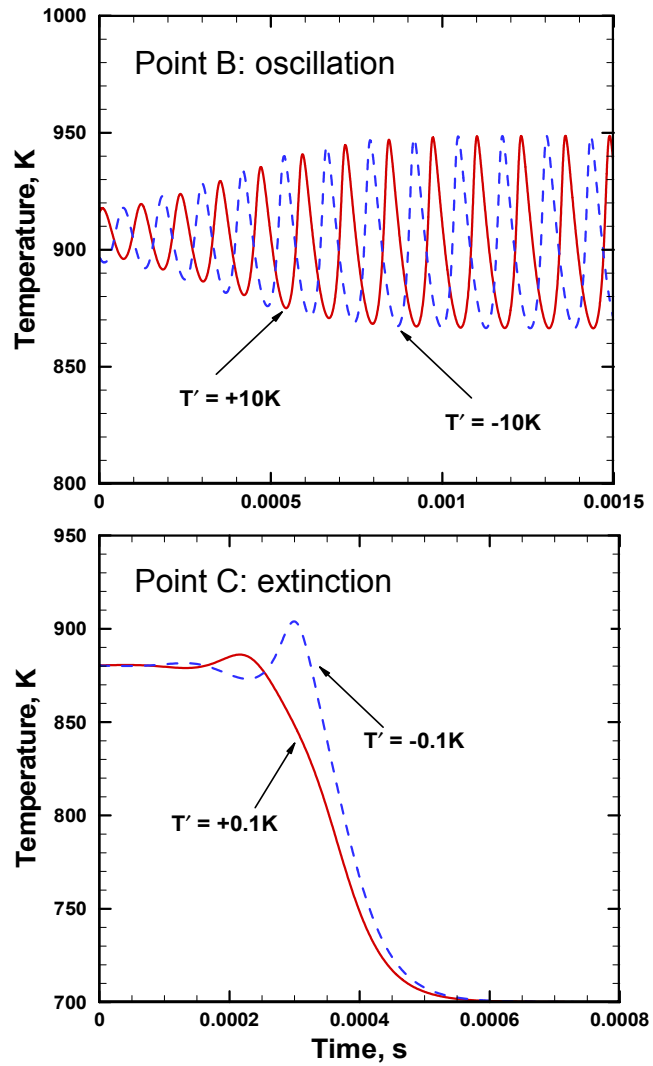


Stable: $\mathrm{Re}(\lambda_1(\mathbf{J}))<0$; Unstable: $\mathrm{Re}(\lambda_1(\mathbf{J}))>0$

- Turning point SE2 is NOT a physical extinction point, SE1 is.

EMA for DME-air (2/3)

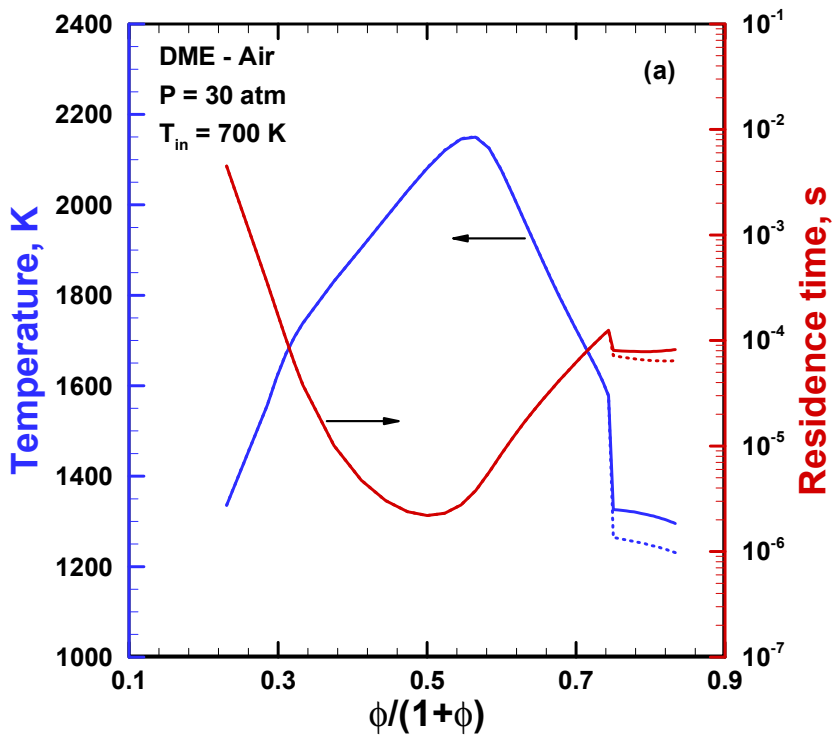




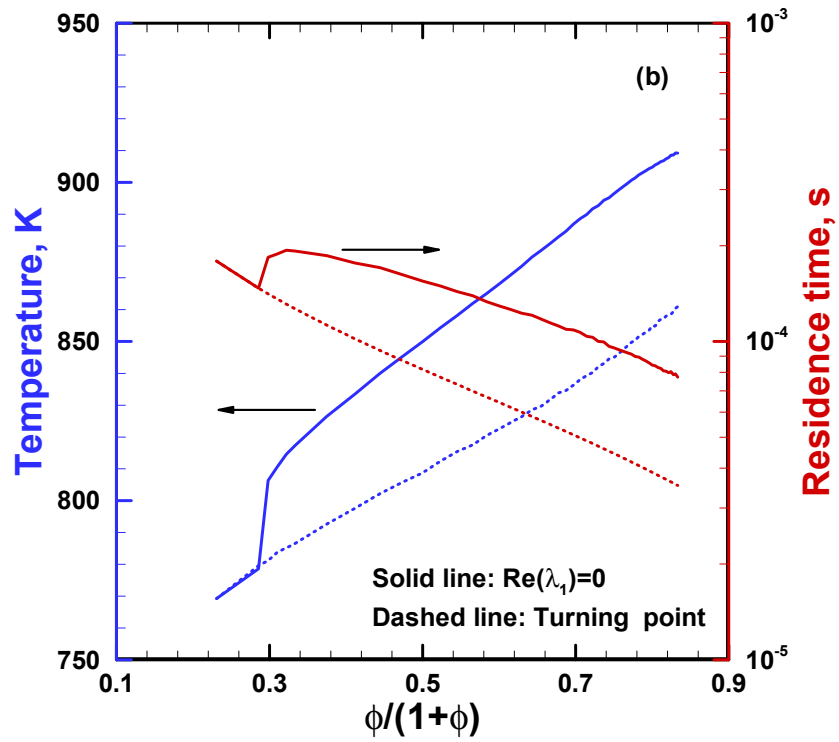
- Turning point CE2 is NOT a physical extinction point
  How about CE1?

EMA for DME-air (3/3)

strong flame extinction



cool flame extinction



- Differences observed for extinction for
  - Rich strong flames; Lean and rich cool flames
- No difference observed for ignition

Summary for EMA

- There can be >2 turning points for fuels with NTC
- Turning points may not be physical ext. or ign. states:

"*Theory must be considered in comparing experimental data*"
- Wing Tsang

- EMA requires analytic Jacobian; difficult for diffusive flames
- Chemical explosive mode analysis (CEMA) (Lu et al 2010) is an efficient alternative for computational flame diagnostics

Part II.

Chemical Explosive Mode Analysis (**CEMA**) for Computational Flame Diagnostics

Chemical Explosive Mode Analysis (CEMA)

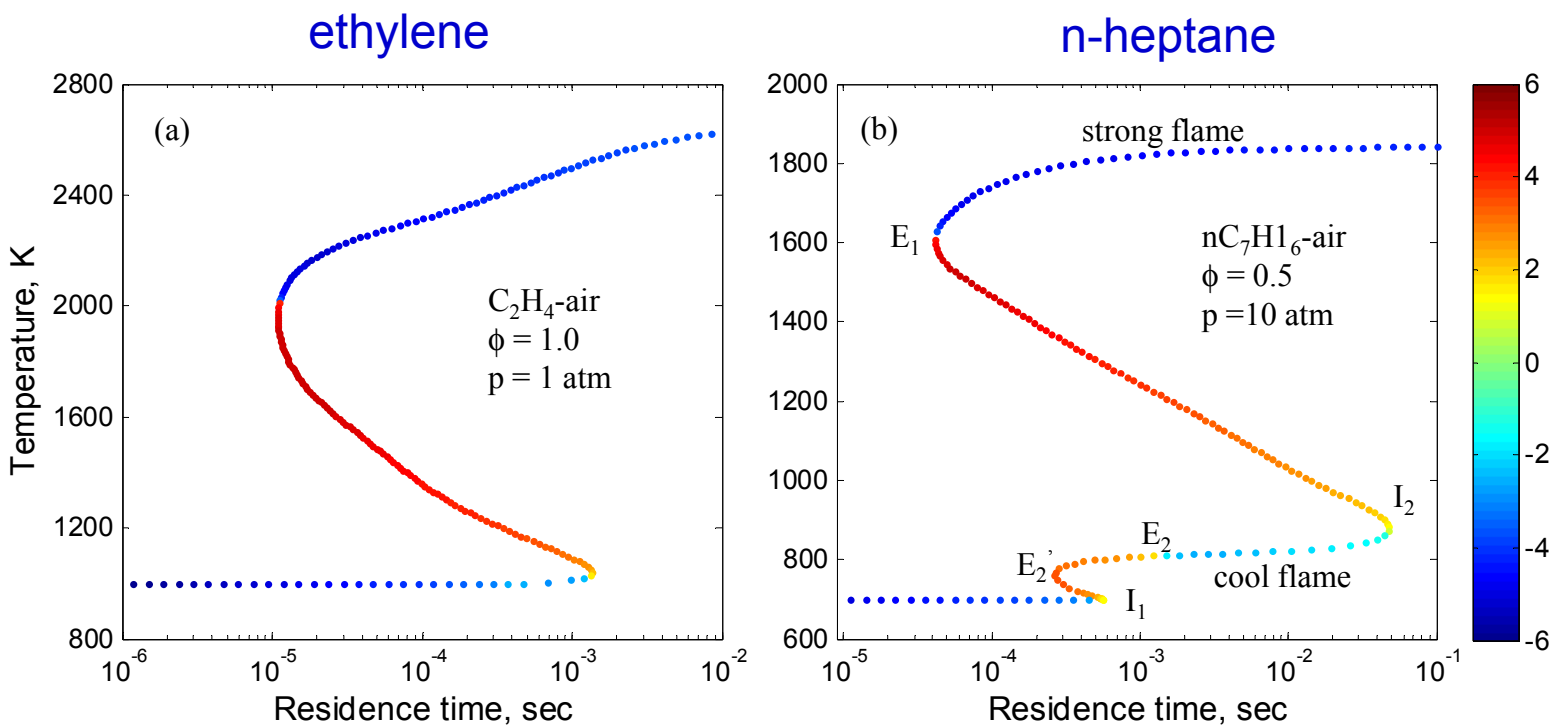
- Governing equations for a chemically reacting flow

$$\frac{d\mathbf{y}}{dt} = \boldsymbol{\omega}(\mathbf{y}) + \mathbf{s}(\mathbf{y})$$

- The chemical Jacobian $\mathbf{J}_{\omega} = \frac{\partial \boldsymbol{\omega}}{\partial \mathbf{y}}$

- chemical explosive mode (CEM): $\mathrm{Re}(\lambda_e)>0$ for $\mathbf{J}_{\omega}$
- CEM indicates the propensity of a mixture to explode when isolated

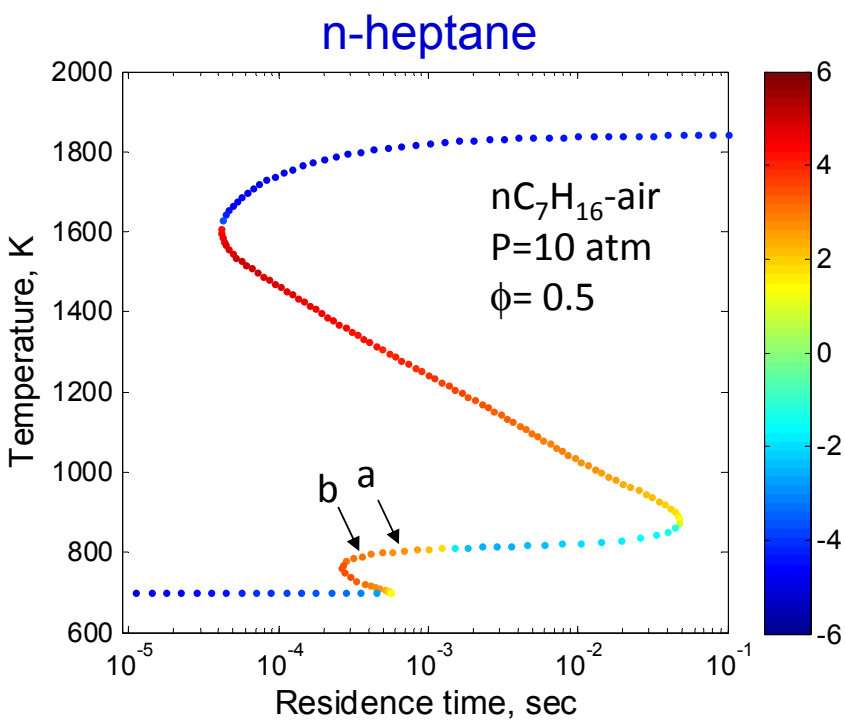
CEMA for Ignition/Extinction in PSR

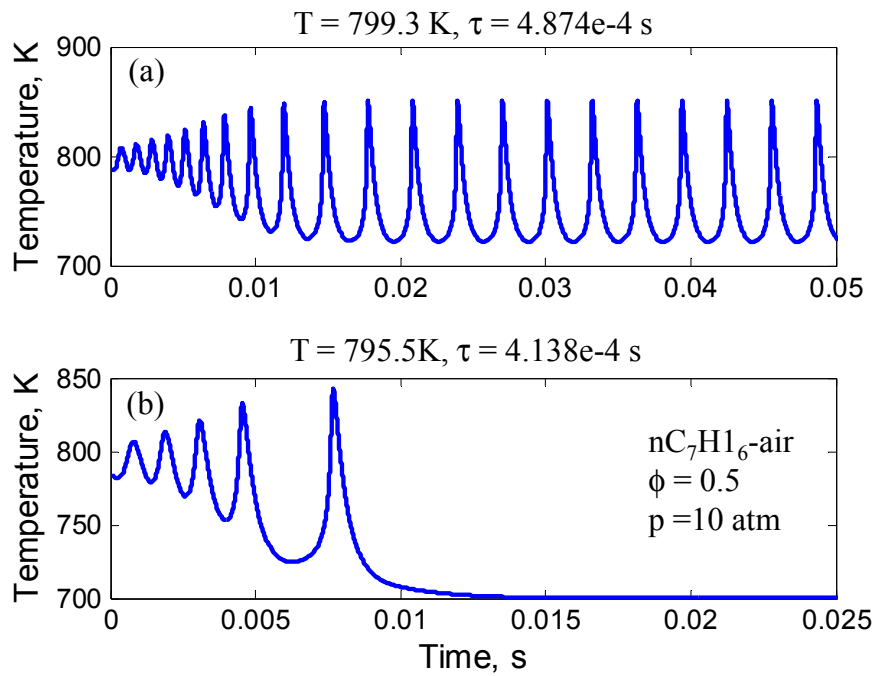


Color indicates $\mathrm{sign}(\mathrm{Re}(\lambda_e)-1/\tau)\times\log_{10}(1+|\mathbf{Re(\lambda_e)-1/\tau}|)$.

- $\mathrm{Re}(\lambda_e)^{-1} \approx \tau$, i.e. CEM balances mixing, at ignition/extinction
- CEM competes with mixing to cause ignition/extinction in steady state systems

Flame Stability based on CEMA

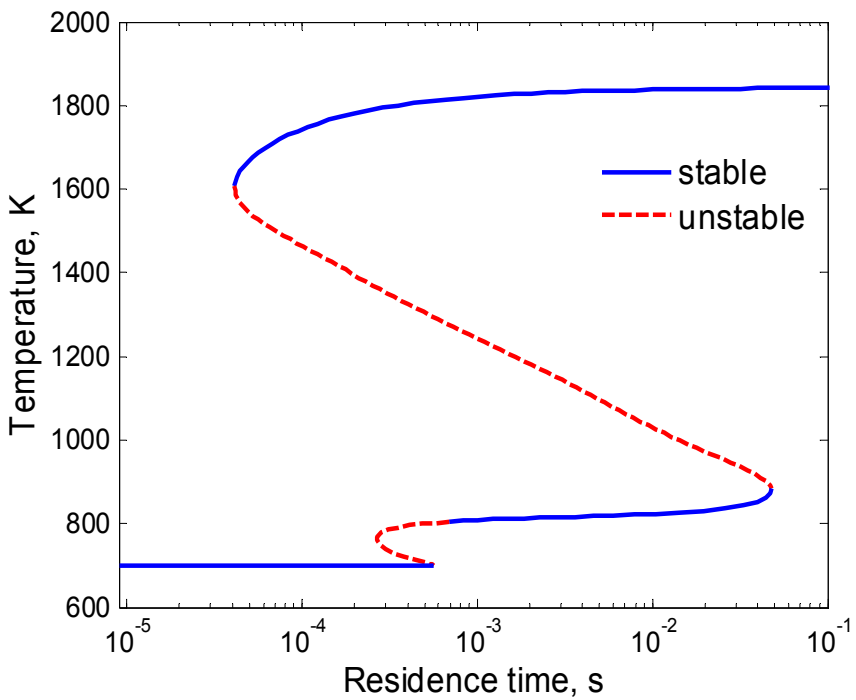




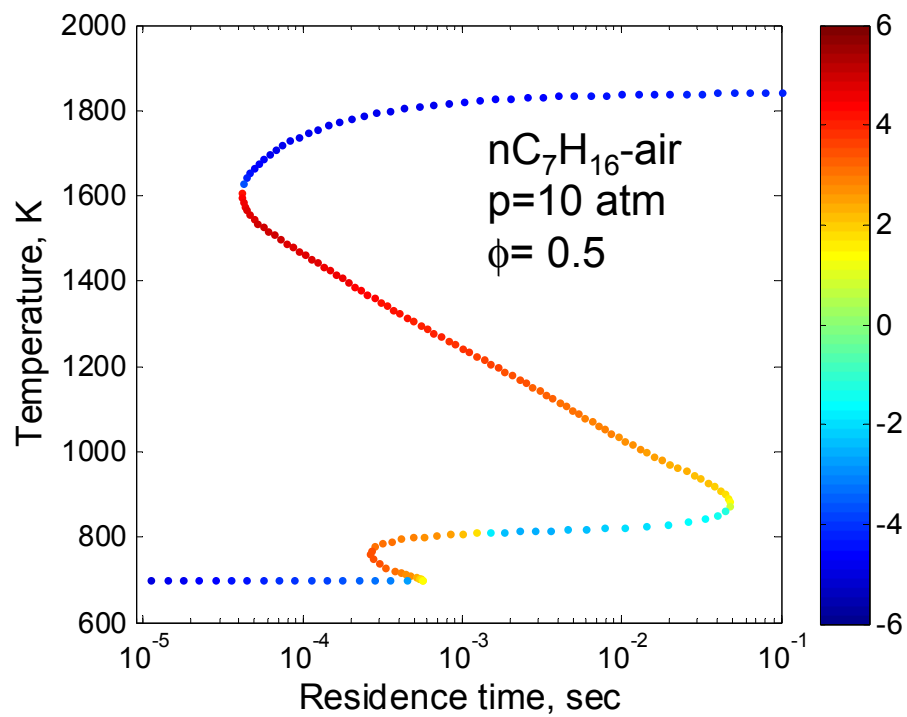
- CEMA result for flame stability highly similar to that of EMA
- Comparison of CEMA & EMA
  - EMA: Jacobian for entire system, high computational cost
  - CEMA: Jacobian for local mixture, computationally efficient

Comparison of EMA and CEMA

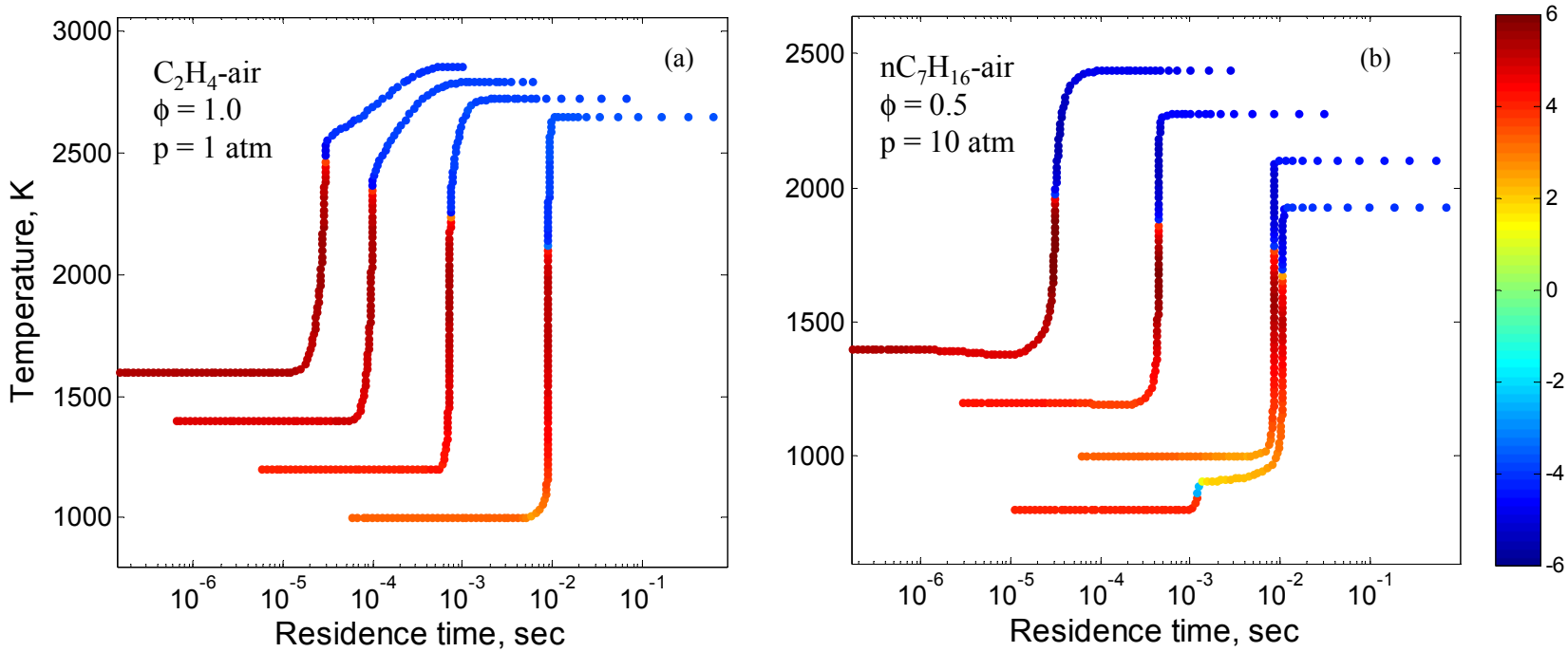
EMA



CEMA



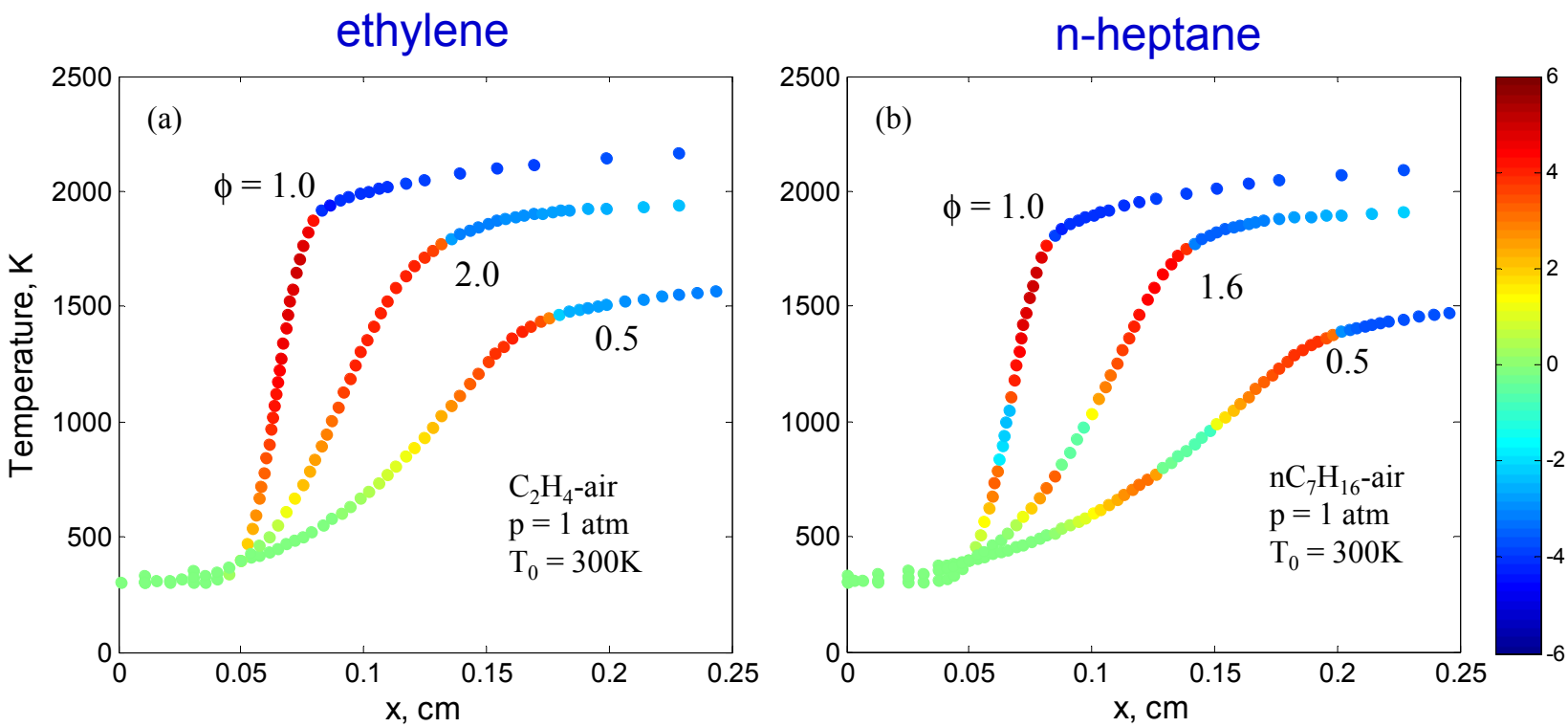
CEMA for Auto-Ignition



Color indicates $\mathrm{sign}(\mathrm{Re}(\lambda_e))\times\log_{10}(1+|\mathbf{Re(\lambda_e)}|)$.

- CEM indicates the propensity of a mixture to explode if isolated
- CEM is present in pre-ignition mixtures; absent in post-ignition mixtures

CEMA for Premixed Flames

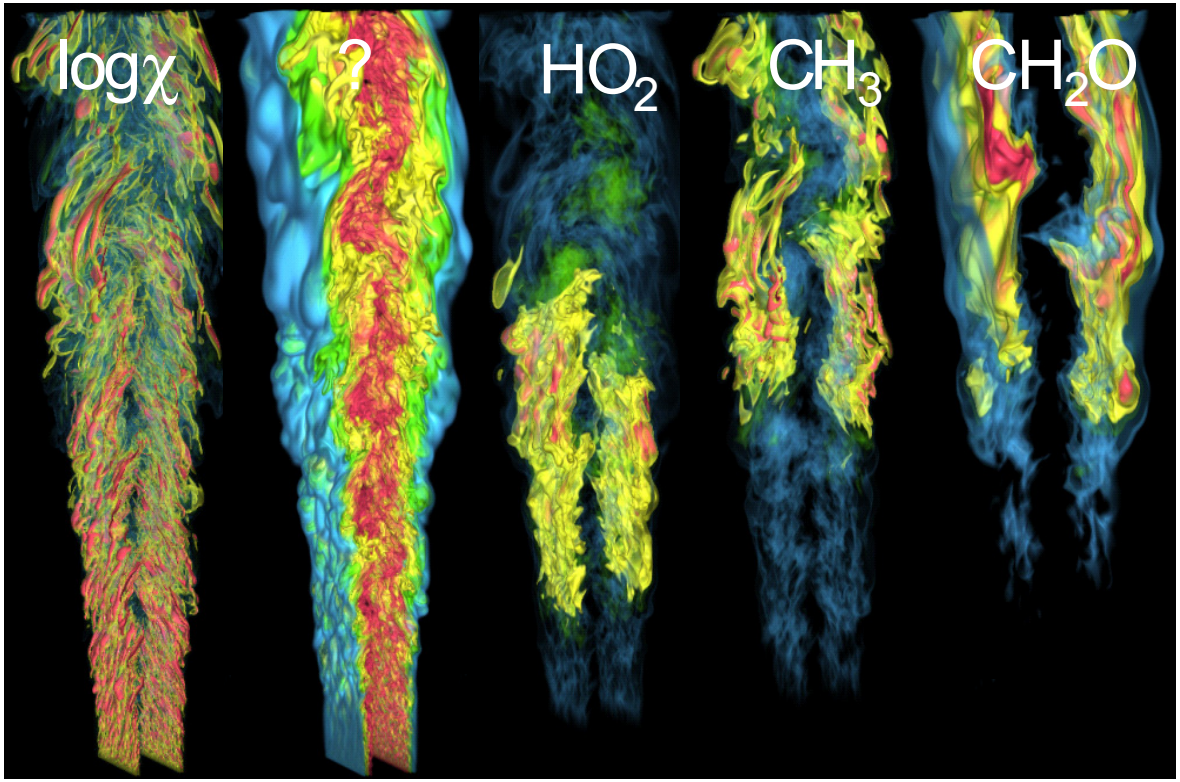


- CEM present for pre-ignition mixtures, absent for post-ignition mixtures (similar to auto-ignition)
- CEM crossover indicates flame front location
- Cool flame zone observed for n-heptane

DNS Data Mining with CEMA: Lifted Ethylene Jet Flame

- 3-D lifted ethylene jet flame (Yoo et al, POCI, 2011)
- 22-species reduced mechanism
- 1.3 billion grid points
- 14 million CPU hours
- 240 TB output

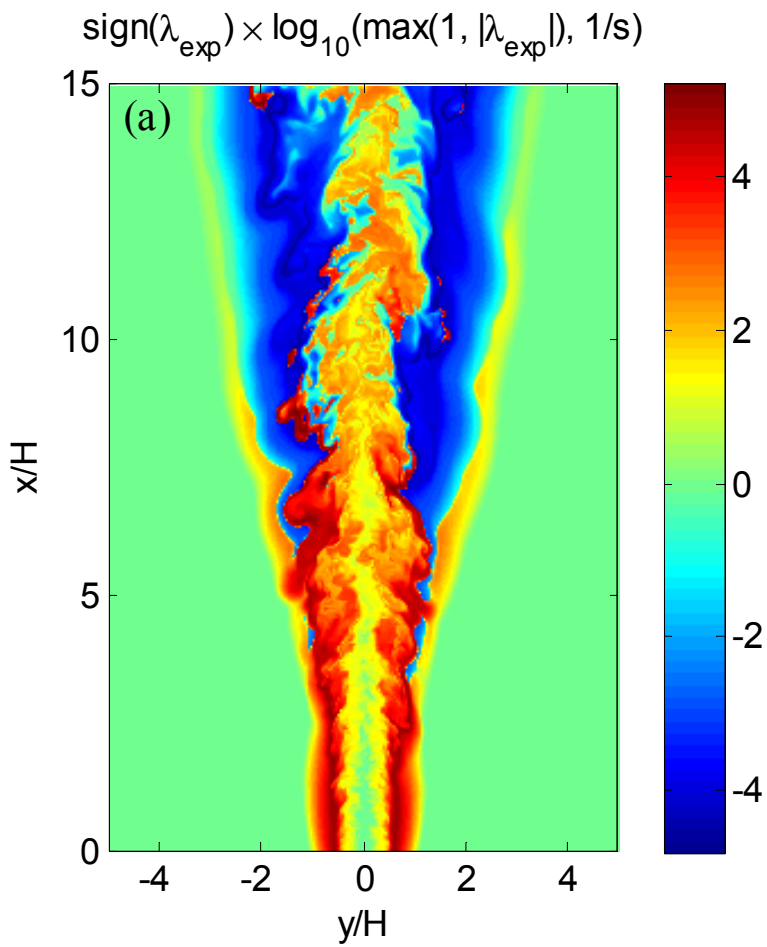
- Fuel: 18% C2H4+82%N2, 550K, 204m/s
- Air: 1550K, 20m/s
- Re: 10000
- Domain size: 30mm x 40mm x 6mm



Volume rendering by H. Yu at Sandia

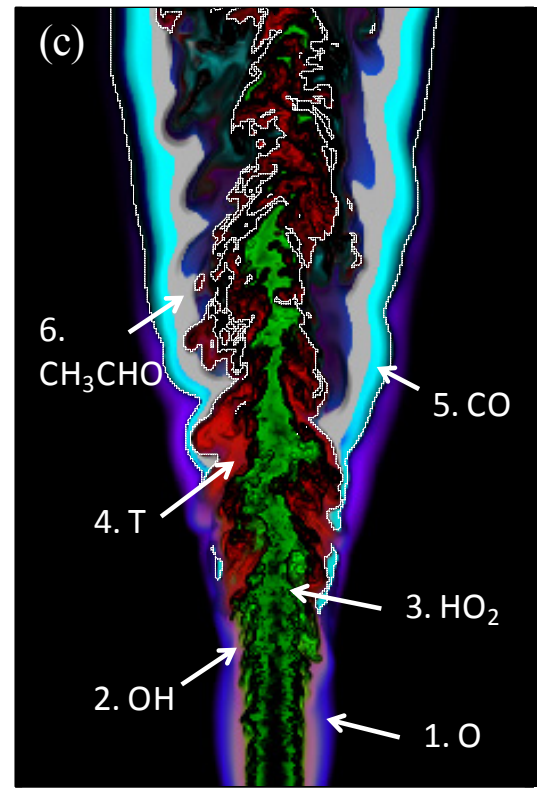
CEMA of the Lifted Ethylene Flame

Time scale



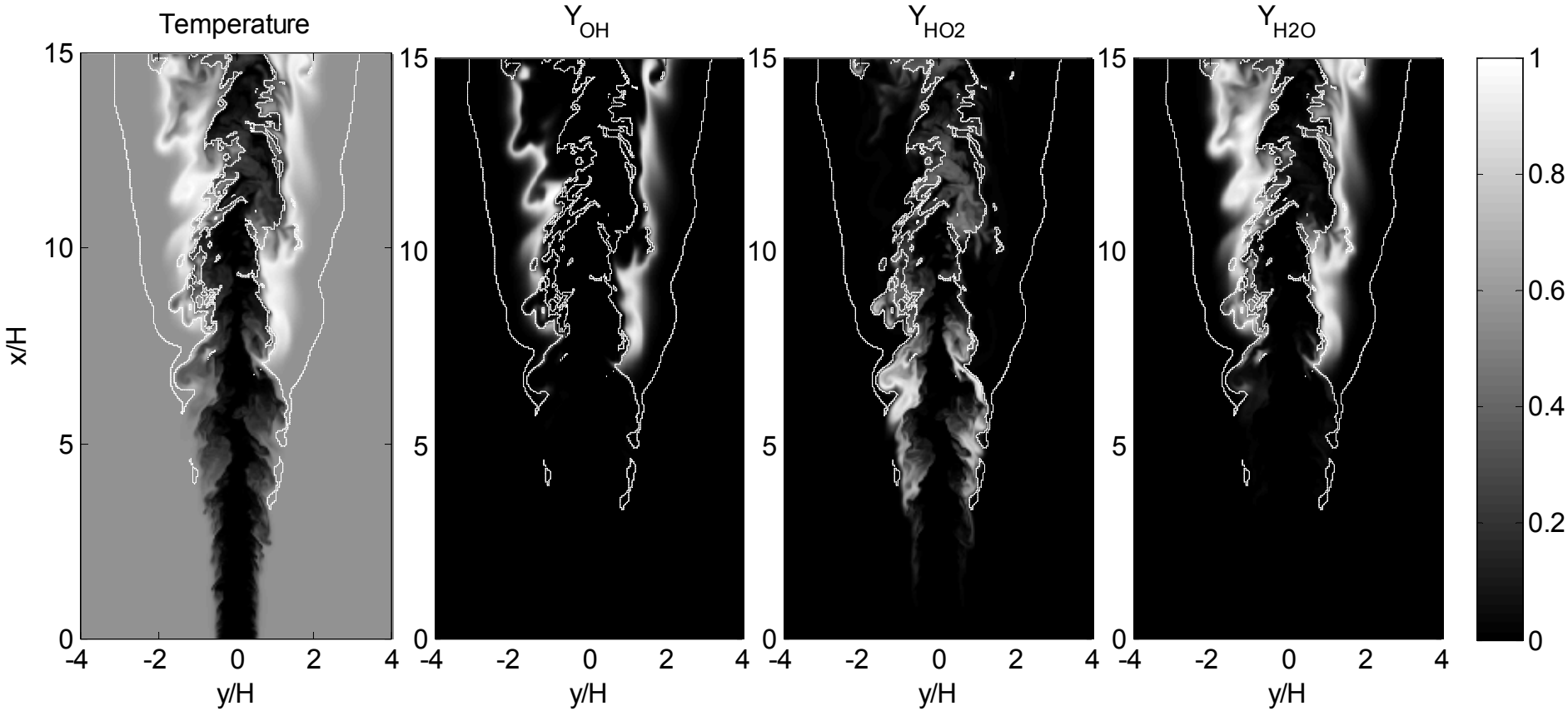
2-D center cut at z = 0
t = 5 flow-through-time

Chemical Structure



$$\mathbf{EI} = \frac{diag\,|\,\mathbf{a}_{\exp}\mathbf{b}_{\exp}\,|}{sum(diag\,|\,\mathbf{a}_{\exp}\mathbf{b}_{\exp}\,|)}$$

CEMA vs. Conventional Scalars



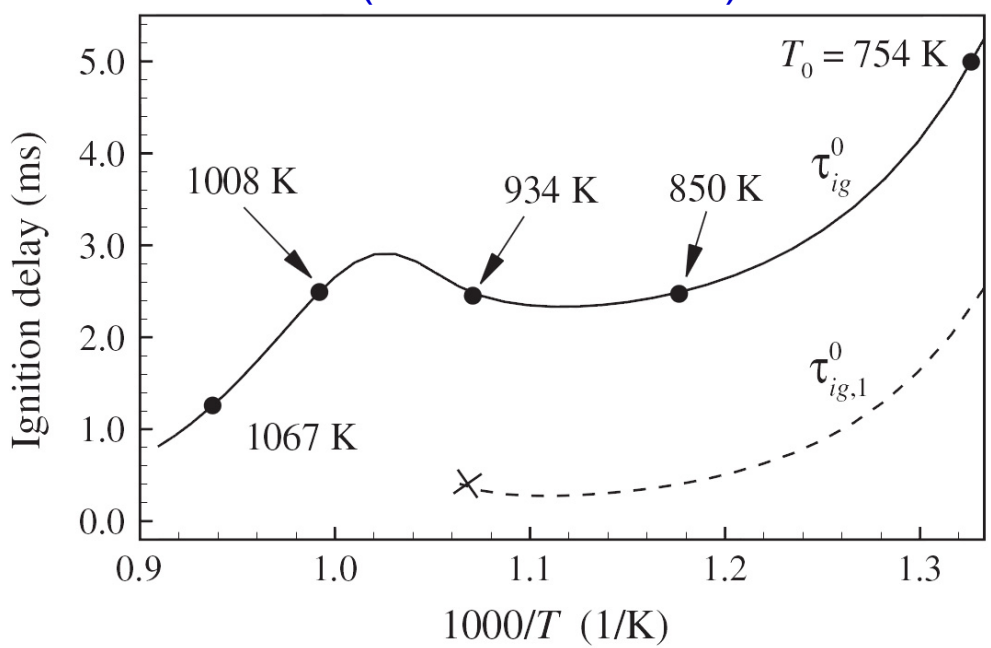
DNS Data Mining with CEMA: 2-D n-heptane-air at HCCI Condition

- 2-D lifted ethylene jet flame (Yoo et al, CNF, 2011)
- 58-species non-stiff reduced mechanism
- Domain size: 3.2mm x 3.2mm
- Grid size: 2.5μm, uniform

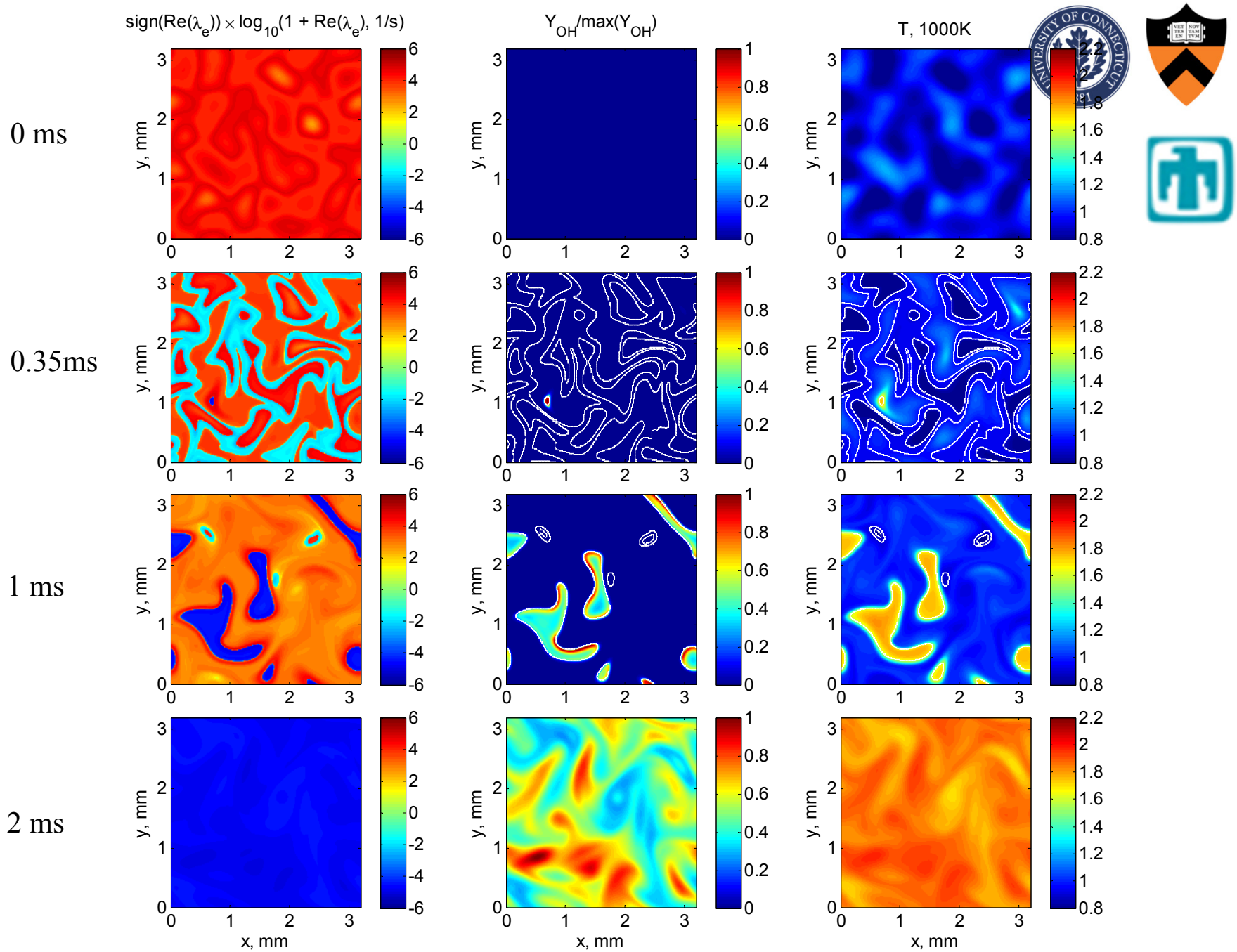
Initial conditions

- ϕ = 0.3
- p = 40 atm
- T_{mean} = 934K, T' = 100K (RMS)
- Isotropic turbulence, u' = 5m/s

Autoignition for n-heptane-air (constant volume)



Play movie here



Summary

- EMA
  - Computational flame diagnostics in system level
  - Flame stability complicated by NTC
- CEMA is a versatile diagnostic for
  - Limit phenomena
  - Premixed flame propagation
  - Chemical structures of flames
- Possible extensions
  - Flame stability in counterflow
  - EMA-guided cool flame ignition/extinction for mechanism validation
  - CEMA for 3-D flame visualization
  - Transport-chemistry interaction by EMA and CEMA

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