On The Model Reduction for Chemical and Physical Kinetics

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Aerothermochemistry and Combustion Systems Laboratory

$SNF - 137771$

PhD Thesis Presentation
18th August 2015

Outline

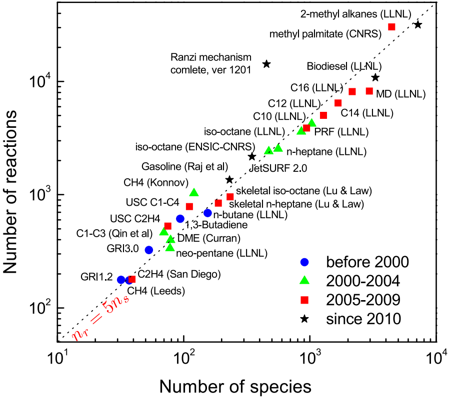
Challenges and Motivation

- ***Every*** Mesh Grid, ***Every*** Time Step
    1. Mass Conservation Equation
    2. Momentum Conservation Equations
    3. Energy Conservation Equation
    4. n_s PDEs for temporal evolution of n_s species

1 Introduction
Motivation
Chem. Kin. Model Reduction
Thesis Outline
2 gRRM
3 Entropy Prod. Ana.
4 n-heptane/air complex dynamics
5 Conclusion

Challenges and Motivation

- ***Every*** Mesh Grid, ***Every*** Time Step
  1. Mass Conservation Equation
  2. Momentum Conservation Equations
  3. Energy Conservation Equation
  4. n_s PDEs for temporal evolution of n_s species
- Size of detailed chemical kinetics



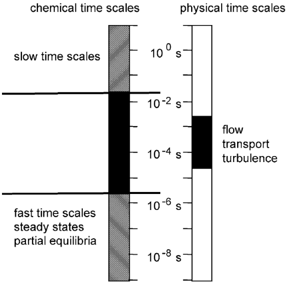
Lu, T., & Law, C. K. (2009). *Prog. Energ. Combust., 35(2)*, 192-215.

	CH_4	C_7H_{16}	$C_{10}H_{22}$	$C_{12}H_{26}$	$C_{20}H_{42}$-2
Species	53	561	940	1282	7200
Reactions	325	2539	3878	5030	31400

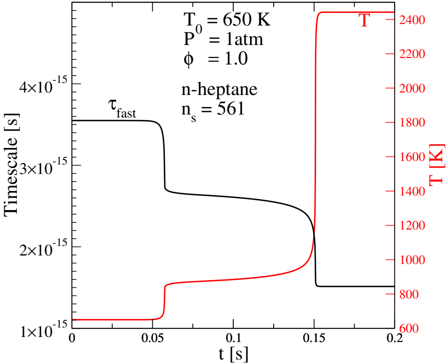
Sizes of detailed reaction mechanisms for sample hydrocarbons

Challenges and Motivation

- ***Every*** Mesh Grid, ***Every*** Time Step
  1. Mass Conservation Equation
  2. Momentum Conservation Equations
  3. Energy Conservation Equation
  4. n_s PDEs for temporal evolution of n_s species
- Stiffness/ Non-linearity



Goussis, D. A., & Maas, U. (2011). In Turbulent Combustion Modeling (pp. 193-220).



Computational Cost Reduction for Chemical Kinetics

A Time scale analysis:

Describe chemistry using fewer variables.

- ✓ **QSSA**: Bodenstein (1913)
- ✓ **CSP**: Lam & Goussis (1989)
- ✓ **ILDM**: Maas & Pope (1992)
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B Conventional Reduction Methodology:

Generate smaller skeletal mechanisms from the detailed mechanism by systematically removing unimportant species and reactions.

- ✓ **CSP**: Massias et al. (1999)
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C Storage and Retrieval methods

- ✓ **ISAT**: Pope (1997)
- ✓ **PRISM**: Tonse (2003)

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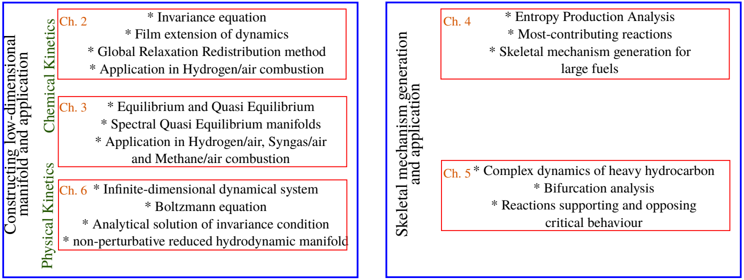

Constructing low-dimensional manifold and application

Chemical Kinetics

Ch. 2
* Invariance equation
* Film extension of dynamics
* Global Relaxation Redistribution method
* Application in Hydrogen/air combustion

Ch. 3
* Equilibrium and Quasi Equilibrium
* Spectral Quasi Equilibrium manifolds
* Application in Hydrogen/air, Syngas/air and Methane/air combustion

Physical Kinetics

Ch. 6
* Infinite-dimensional dynamical system
* Boltzmann equation
* Analytical solution of invariance condition
* non-perturbative reduced hydrodynamic manifold

Skeletal mechanism generation and application

Ch. 4
* Entropy Production Analysis
* Most-contributing reactions
* Skeletal mechanism generation for large fuels

Ch. 5
* Complex dynamics of heavy hydrocarbon
* Bifurcation analysis
* Reactions supporting and opposing critical behaviour

Thesis in a nutshell

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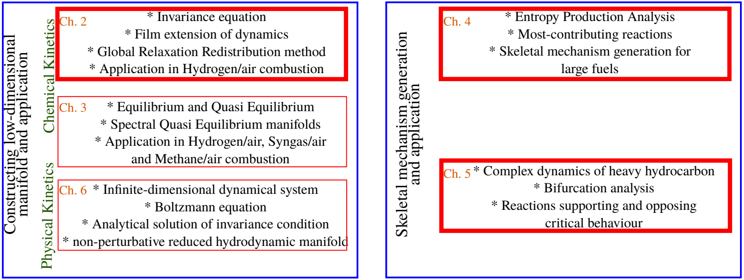

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Thesis in a nutshell

II. The global Relaxation Redistribution Method

Concept of Slow Invariant Manifold

Classification of Systems

- Autonomous system
- Cauchy-Lipschitz

$$\frac{d\mathbf{N}}{dt} = \boldsymbol{f}(\mathbf{N})$$

$$\boldsymbol{f} : \mathbb{R}^{n_s} \supset S \to \mathbb{R}^{n_s}$$

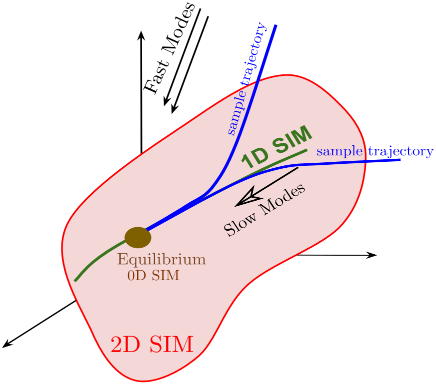
$$\mathbf{N} \in S, t \in \mathbb{T}$$

$\phi^t{}_{t\in\mathbb{T}}$ is called a flow where

$$\mathbf{N}_t = \phi^t \mathbf{N}_0$$

$\mathbf{N}^{eq}$ is a unique fixed point.

- In dynamical system $\{\mathbb{T}, S, \phi^t\}$, $U \subset S$ is invariant manifold (set) if $N_0 \in U$ then $\forall t$: $\phi^t \mathbf{N}_0 \in U$
- Slow Invariant Manifold (SIM)



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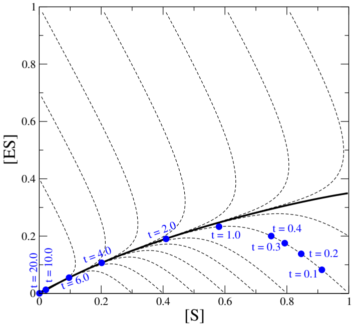


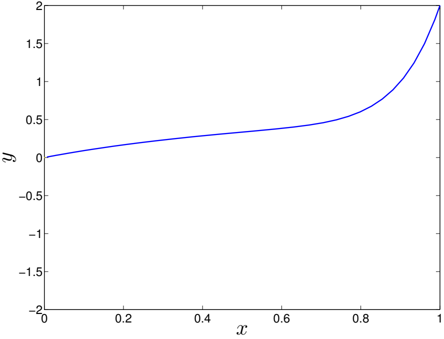
$$\mathrm{S} + \mathrm{E} \underset{\mathrm{k_{r1}}}{\overset{\mathrm{k_{f1}}}{\rightleftharpoons}} \mathrm{ES} \xrightarrow{\mathrm{k_{cat}}} \mathrm{E} + \mathrm{P}$$

$$k_{1f} = k_{1r} = k_{cat} = 1$$

Multiscale Dissipation

Davis-Skodje System (J. Chem. Phys. 1999):

$$\begin{cases} \frac{dx}{dt} = -x \\ \frac{dy}{dt} = -\gamma y + \frac{(\gamma-1)x+\gamma x^2}{(1+x)^2} \\ \gamma \gg 1, \gamma = 5 \end{cases}$$



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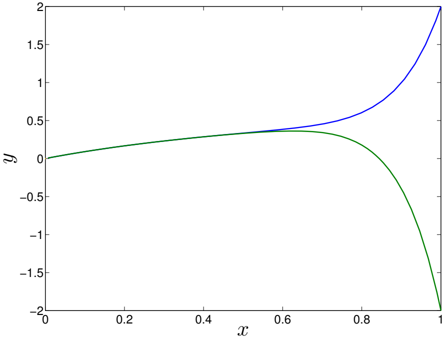

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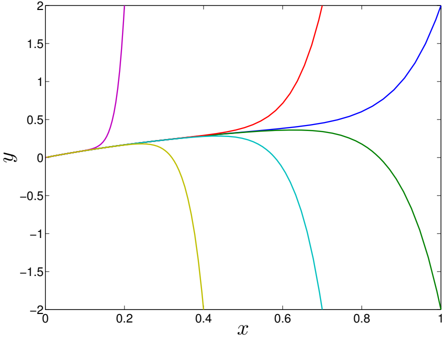

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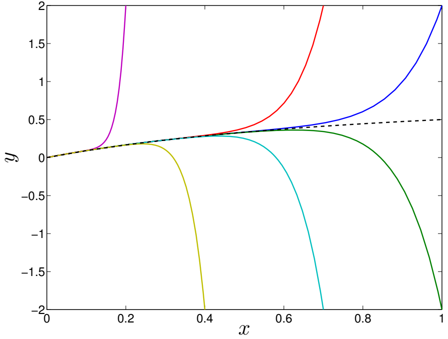

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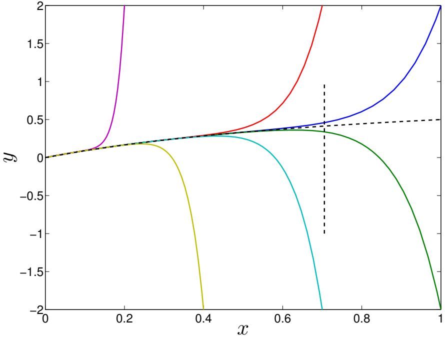

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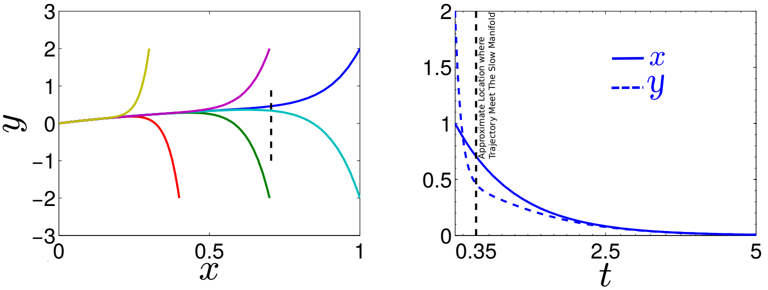

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$$x = x_0 e^{-t}$$

$$y = \frac{x_0 e^{-t}}{1 + x_0 e^{-t}} + \cancelto{0}{C(x_0, y_0) e^{-\gamma t}}$$

$$y_{slow} = \frac{x}{1+x}$$

Multiscale Dissipation

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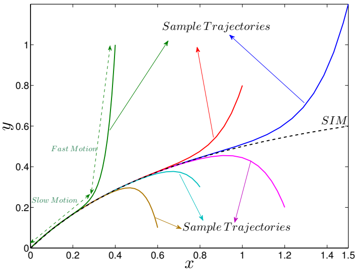
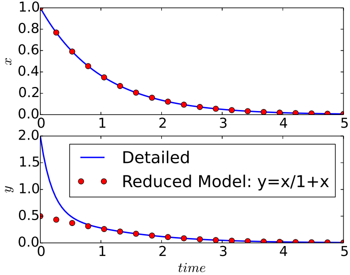
$$\begin{cases} \dfrac{dx}{dt} = -x \\ \dfrac{dy}{dt} = -\gamma y + \dfrac{(\gamma-1)x+\gamma x^2}{(1+x)^2} \\ \gamma \gg 1 \\ \Longrightarrow y_{SIM} = \dfrac{x}{1+x} \end{cases}$$





Method of Invariant Manifold (MIM)

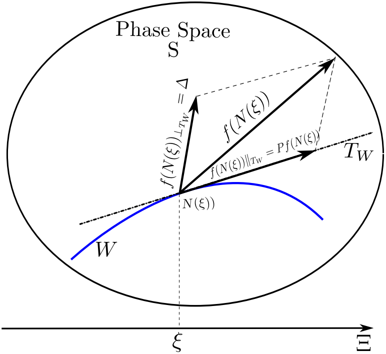
$$\boldsymbol{f}(\mathbf{N}(\xi)) = \boldsymbol{f}(\mathbf{N}(\xi))_{\|_{T_W}} + \boldsymbol{f}(\mathbf{N}(\xi))_{\perp_{T_W}}$$

$$\boldsymbol{f}(\mathbf{N}(\xi))_{\|_{T_W}} = \mathbf{P}\boldsymbol{f}(\mathbf{N}(\xi))$$

$$\boldsymbol{f}(\mathbf{N}(\xi))_{\perp_{T_W}} = \Delta = (\mathbf{I} - \mathbf{P})\boldsymbol{f}(\mathbf{N}(\xi))$$

Invariance Condition

$$\Delta = 0, \qquad \xi \in \Xi$$



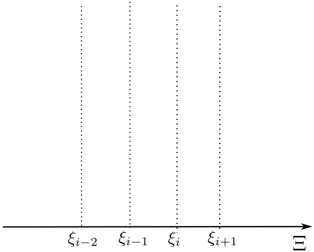
MIM: The slow invariant manifold is the stable solution of the film extension of dynamics:

$$\frac{d\mathbf{N}(\xi)}{dt} = \Delta$$

Gorban, A. N., & Karlin, I. V. (2004). *Lect. Notes Phys.*, 660.

Relaxation Redistribution Method (RRM)

1. Find/Choose the slow parameterization variables



Chiavazzo, E., & Karlin, I. V. (2011). *Phys. Rev. E*, *83*(3), 036706.
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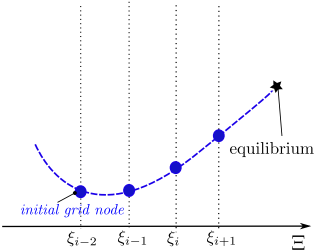
1. Find/Choose the slow parameterization variables
2. Construct the initial guess of slow manifold



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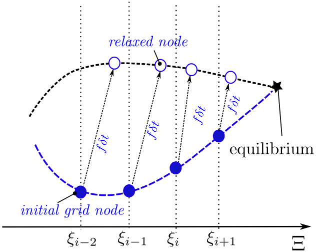

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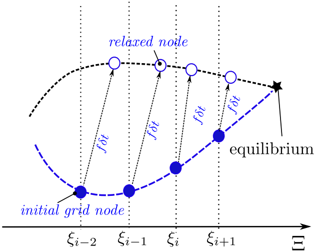
4. Points moving toward local equilibrium manifold



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1. Find/Choose the slow parameterization variables
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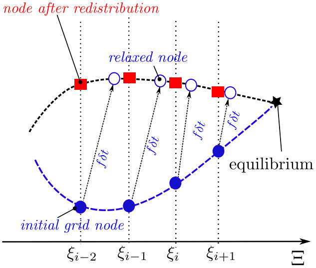
4. Points moving toward local equilibrium manifold
5. Redistribute back to neutralize slow motion
    - Redistribution : Interpolation for interior
    - Redistribution : Extrapolation for missing point



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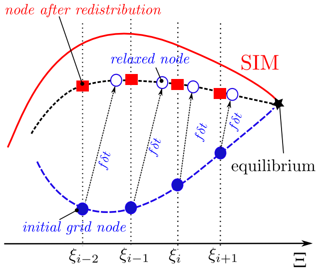

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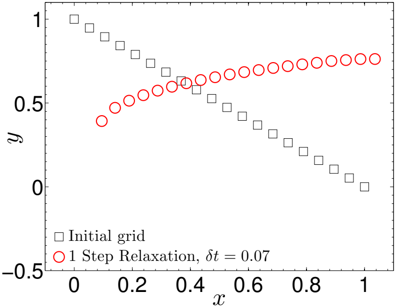
RRM Manifold Construction

Singular perturbed system*

$$\begin{cases} \frac{dx}{dt} = 2 - x - y \\ \frac{dy}{dt} = \gamma(\sqrt{x} - y) \\ \gamma \gg 1 \end{cases}$$

Relaxation Step



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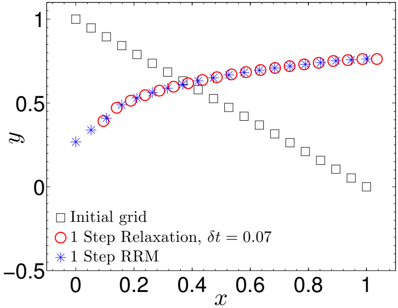
Redistribution Step



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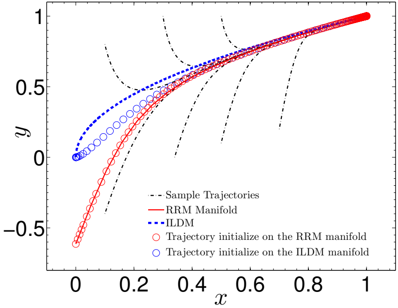
- ILDM manifold is neither invariant nor slow for $0 \leq x \lesssim 0.7$.



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Dimensionality issues

- Computational cost
  - Manifolds are represented on a grid
  - Retrieving data of high dimensional tables, imposes restrictions on the dimension

$\Longrightarrow$ Target : 2D/3D manifold

Pope, S. B. (2013). *Proc. Combust. Inst., 34(1)*, 1-31.

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$\Longrightarrow$ Target : 2D/3D manifold

- Dimension of SIMs
  - SIMs usually limited to a small neighborhood around equilibrium

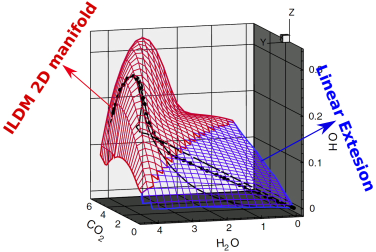
$\Longrightarrow$ How to extend it further to cover the states all the way to the fresh mixture?

Pope, S. B. (2013). *Proc. Combust. Inst., 34(1)*, 1-31.

Dimensionality issues

⟹ How to extend it further to cover the states all the way to the fresh mixture?

- Construct the Slow invariant manifold and extend via prolongation with linear extrapolation*



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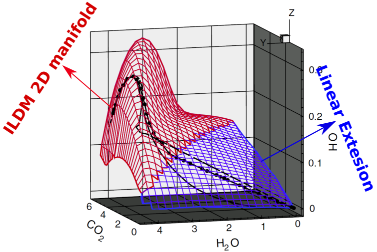

- Construct the initial grid which covers the admissible solution space and refine it via RRM, (global RRM**)

*Bykov, V., & Maas, U. (2007). *Proc. Combust. Inst., 31(1)*, 465-472.
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Constructing Manifold
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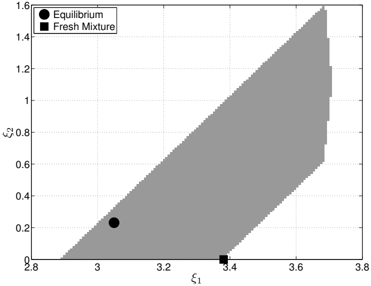
2. Find the boundaries of initial grid



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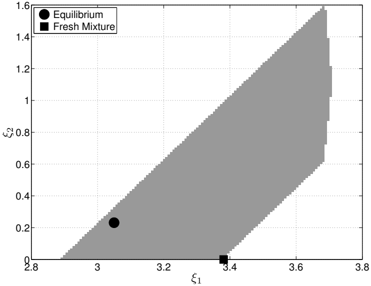

3. Relax interior points
4. Redistribute back points on initial grid via interpolation of scattered grid

global RRM (gRRM)

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- The n_d-dimensional SIM +
- The extension of SIM to the far from equilibrium states

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The gRRM n_d-dimensional manifold is:

- The n_d-dimensional SIM +
- The extension of SIM to the far from equilibrium states

$\Longrightarrow$ The initial grid is important both for convergence and accuracy of extension

$\Longrightarrow$ In this work the initial grid is found based on notation of Quasi Equilibrium Manifold (QEM)

Initial Grid via QEM (CEM)

$$\begin{array}{ll} \min & G \\ \text{s.t.} & \mathbf{BN} = \xi \end{array}$$

$$\mathbf{B} = [\mathbf{E}\ \mathbf{B}^d] \text{ and } \xi = [\xi^e\ \xi^d]$$

- $n_e \times n_s$ elemental constraints matrix, $\mathbf{E}$

$$\mathbf{EN} = \xi^e$$

  ξ^e is specified by the initial composition
  E_{ji} : number of atoms of element j in species i

- $n_d \times n_s$ constraints matrix $\mathbf{B}^d$

$$(\mathbf{B}^d)\mathbf{N} = \xi^d$$

  ξ^d : slow parameters
  $\mathbf{B}^d$: rows define the linear combination of $\mathbf{N}$ as the slow constraints

Manifold parametrization Ξ / Proper choose for extension

How to Choose a good set of constraints $\mathbf{B}^d$?

- Rate-Controlled Constrained-Equilibrium method (RCCE)
- constraints for H_2/air combustion with $n_s = 9$ species and $n_r = 21$ elementary reactions*

Reduce Parameter**	H_2	N_2	H	O	OH	O_2	H_2O	HO_2	H_2O_2
ξ_1=Total Mole	1	1	1	1	1	1	1	1	1
ξ_2=Active Valence	0	0	1	2	1	0	0	0	0
ξ_3=Free Oxygen	0	0	0	1	1	0	1	0	0

$$\mathbf{B}^d = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

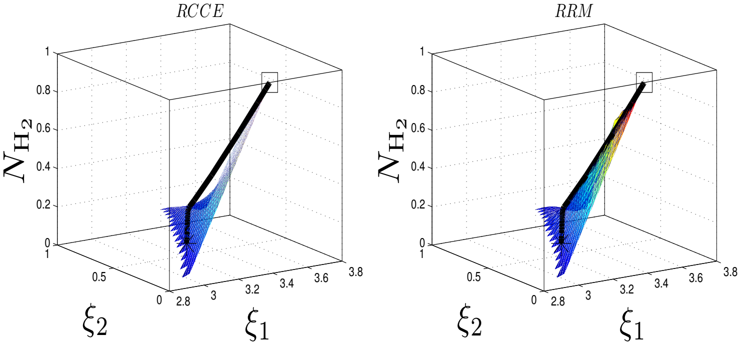
---

*Li, J., et al., (2004). *Int. J. Chem. Kin.*, 36(10), 566-575.

**Tang, Q., & Pope, S. B. (2004). *Combust. Theory Model.*, 8(2), 255-279.

gRRM for H_2/air combustion

$n_s = 9$ Species, $T_0 = 1500\,K$, $P = 1\,atm$, $\phi = 1.0$



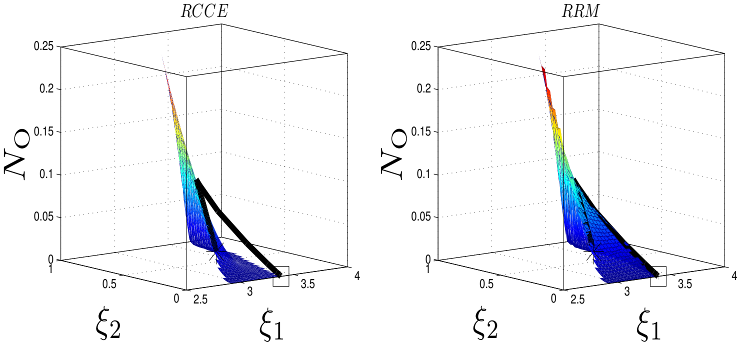
ξ_1=Total Mole, ξ_2=Active Valence

Slight improvements in main species

□, fresh mixture; ⋆ , equilibrium point; – detailed kinetics path, Colored surfaces, Manifolds

gRRM for H_2/air combustion

$n_s = 9$ Species, $T_0 = 1500\,K$, $P = 1\,atm$, $\phi = 1.0$



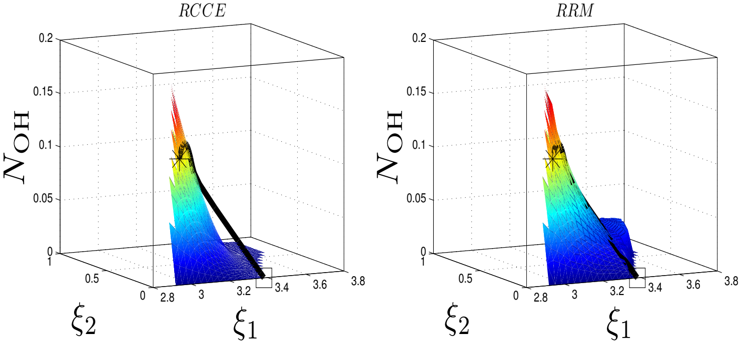
ξ_1=Total Mole, ξ_2=Active Valence

Small improvements in main radicals

☐, fresh mixture; $\star$, equilibrium point; $-$ detailed kinetics path, Colored surfaces, Manifolds

gRRM for H_2/air combustion

$n_s = 9$ Species, $T_0 = 1500\,K$, $P = 1\,atm$, $\phi = 1.0$



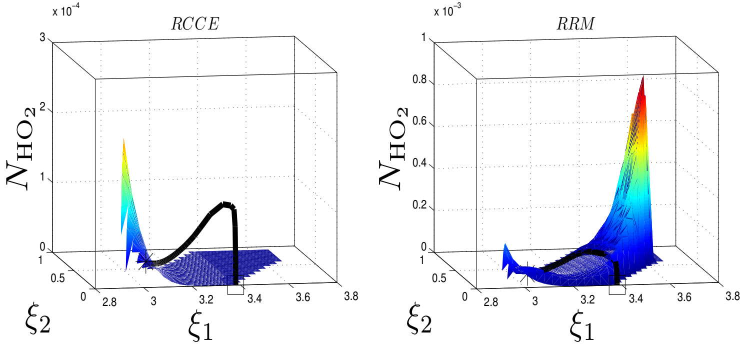
ξ_1=Total Mole, ξ_2=Active Valence

Small improvements in main radicals

☐, fresh mixture; $\star$, equilibrium point; $-$ detailed kinetics path, Colored surfaces, Manifolds

gRRM for H_2/air combustion

$n_s = 9$ Species, $T_0 = 1500\,K$, $P = 1\,atm$, $\phi = 1.0$



ξ_1=Total Mole, ξ_2=Active Valence

Large improvements for low-concentration radicals

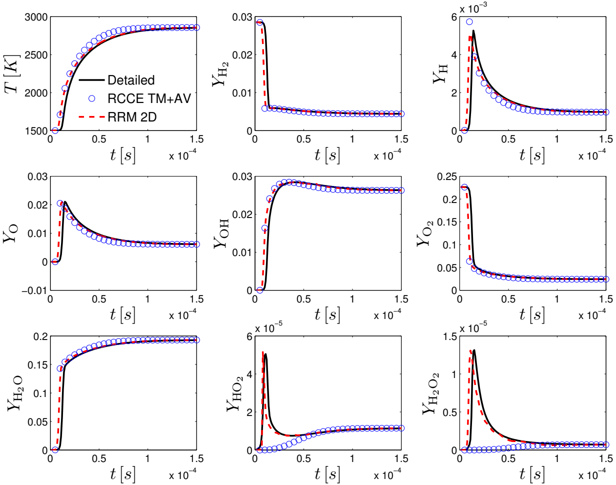
□, fresh mixture; $\star$, equilibrium point; $-$ detailed kinetics path, Colored surfaces, Manifolds

H_2/air auto-ignition

Adiabatic, constant pressure reactor

$T_0 = 1500\,K$, $P = 1\,atm$, $\phi = 1.0$

2D manifold results

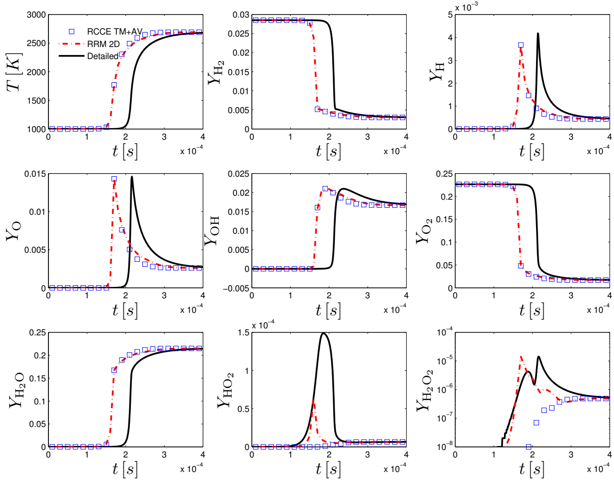


H_2/air auto-ignition

Adiabatic, constant pressure reactor

$T_0 = 1000\,K$, $P = 1\,atm$, $\phi = 1.0$

2D manifold results

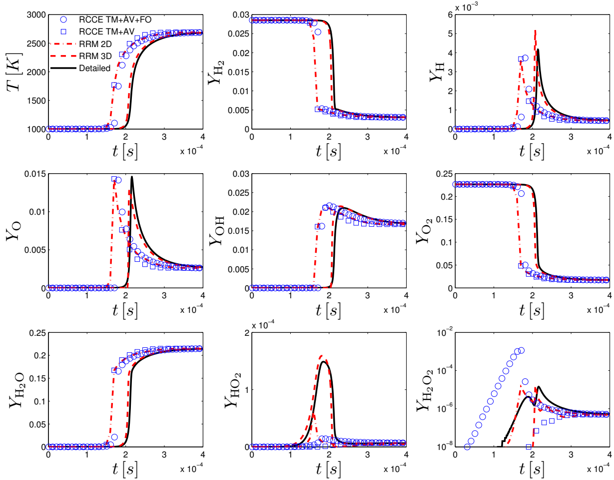


H_2/air auto-ignition

Adiabatic, constant pressure reactor

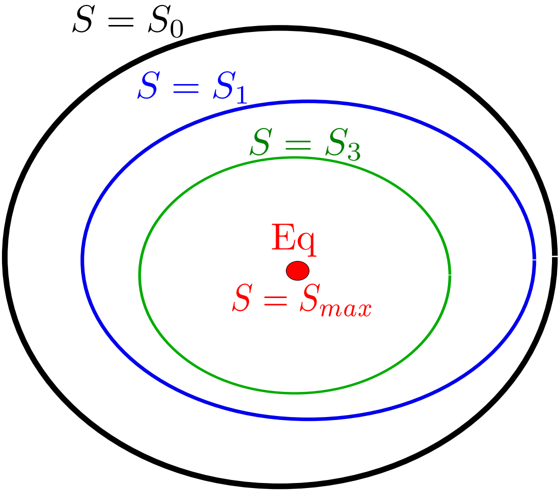
$T_0 = 1000\,K$, $P = 1\,atm$, $\phi = 1.0$

3D manifold results

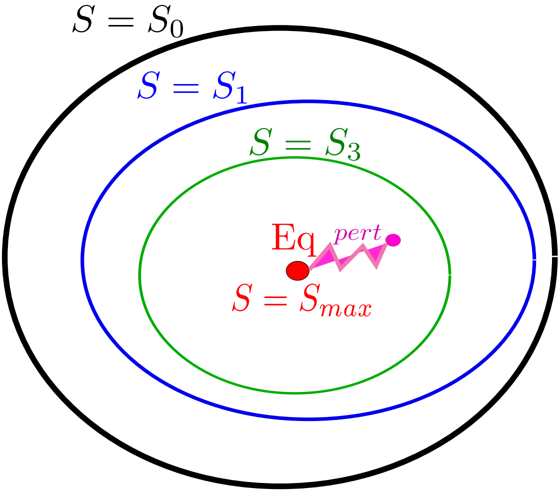


III. Entropy production analysis for mechanism reduction

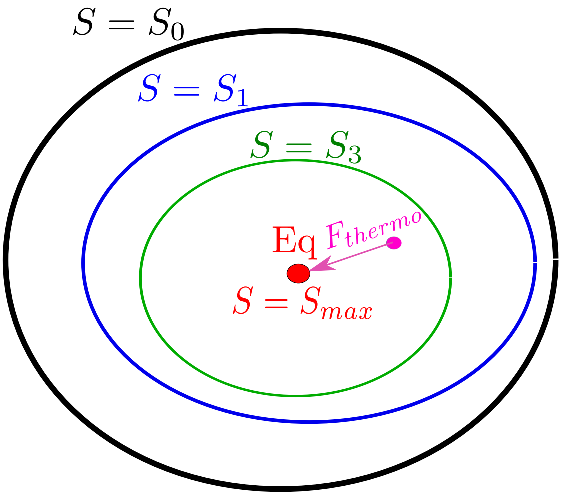
Entropy Production



Entropy Production



Entropy Production



Entropy Production

$$\sum_{i=1}^{n_s} \nu'_{ik} N_i \rightleftharpoons \sum_{i=1}^{n_s} \nu''_{ik} N_i, \quad k = 1, \cdots, n_r$$

$$q_k = q_{f_k} - q_{r_k} = k_{f_k} \prod_{i=1}^{n_s} [N_i]^{\nu'_{ik}} - k_{r_k} \prod_{i=1}^{n_s} [N_i]^{\nu''_{ik}}, \quad k = 1, \cdots, r$$

The entropy production per unit volume

$$\frac{1}{V}\frac{dS}{dt} = R_c \sum_{k=1}^{n_r} (q_{f_k} - q_{r_k}) ln \left(\frac{q_{f_k}}{q_{r_k}} \right)$$

The relative contribution of each reaction in total entropy production at time t

$$r_k(t) = \frac{R_c (q_{f_k} - q_{r_k}) ln \left(\frac{q_{f_k}}{q_{r_k}} \right)}{\frac{1}{V}\frac{dS}{dt}}$$

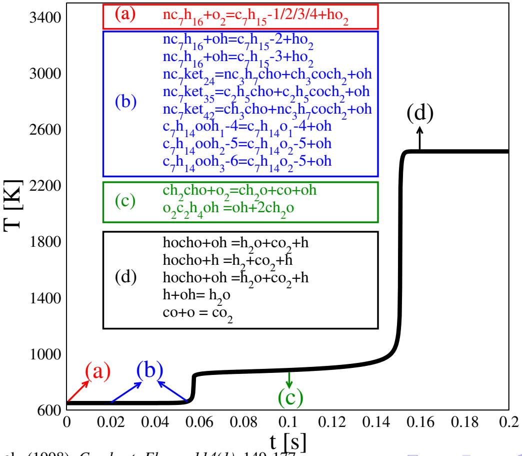
Threshold for contribution

$$r_k(t) \geq \varepsilon\%$$

Most-Contributing Reactions

n-heptane LLNL2 Mechanism ($n_s = 561$, $n_r = 2539$)*
$T_0 = 650$ K, $P = 1$ atm, $\phi = 1$

$\varepsilon = 5\%$



*Curran, H. J., et al., (1998). *Combust. Flame, 114(1)*, 149-177.

Generate Skeletal Mechanism

Most-contributing reactions

$\boxed{nc_7h_{16}}+o_2=\boxed{c_7h_{15}\text{-}1/2/3/4}+\boxed{ho_2}$

$nc_7h_{16}+oh=c_7h_{15}\text{-}2+ho_2$
$nc_7h_{16}+oh=c_7h_{15}\text{-}3+ho_2$
$\boxed{nc_7ket_{24}}=\boxed{nc_3h_7cho}+\boxed{ch_3coch_2}+oh$
$\boxed{nc_7ket_{35}}=\boxed{c_2h_5cho}+\boxed{c_2h_5coch_2}+oh$
$\boxed{nc_7ket_{42}}=\boxed{ch_3cho}+\boxed{nc_3h_7coch_2}+oh$
$\boxed{c_7h_{14}ooh_1\text{-}4}=\boxed{c_7h_{14}o_1\text{-}4}+\boxed{oh}$
$\boxed{c_7h_{14}ooh_2\text{-}5}=\boxed{c_7h_{14}o_2\text{-}5}+oh$
$\boxed{c_7h_{14}ooh_3\text{-}6}=\boxed{c_7h_{14}o_2\text{-}5}+oh$

$\boxed{ch_2cho}+o_2=ch_2o+\boxed{co}+oh$
$\boxed{o_2c_2h_4oh}=oh+2\boxed{ch_2o}$

$\boxed{hocho}+oh=\boxed{h_2o}+\boxed{co_2}+\boxed{h}$
$hocho+h=\boxed{h_2}+co_2+h$
$hocho+oh=h_2o+co_2+h$
$h+oh=h_2o$
$co+\boxed{o}=co_2$

Generate Skeletal Mechanism

Most-contributing reactions

$\boxed{nc_7h_{16}}+o_2=\boxed{c_7h_{15}\text{-}1/2/3/4}+\boxed{ho_2}$

$nc_7h_{16}+oh=c_7h_{15}\text{-}2+ho_2$
$nc_7h_{16}+oh=c_7h_{15}\text{-}3+ho_2$
$\boxed{nc_7ket_{24}}=\boxed{nc_3h_7cho}+\boxed{ch_3coch_2}+oh$
$\boxed{nc_7ket_{35}}=\boxed{c_2h_5cho}+\boxed{c_2h_5coch_2}+oh$
$\boxed{nc_7ket_{42}}=\boxed{ch_3cho}+\boxed{nc_3h_7coch_2}+oh$
$\boxed{c_7h_{14}ooh_1\text{-}4}=\boxed{c_7h_{14}o_1\text{-}4}+\boxed{oh}$
$\boxed{c_7h_{14}ooh_2\text{-}5}=\boxed{c_7h_{14}o_2\text{-}5}+oh$
$\boxed{c_7h_{14}ooh_3\text{-}6}=\boxed{c_7h_{14}o_2\text{-}5}+oh$

$\boxed{ch_2cho}+o_2=ch_2o+\boxed{co}+oh$
$\boxed{o_2c_2h_4oh}=oh+2\boxed{ch_2o}$

$\boxed{hocho}+oh=\boxed{h_2o}+\boxed{co_2}+\boxed{h}$
$hocho+h=\boxed{h_2}+co_2+h$
$hocho+oh=h_2o+co_2+h$
$h+oh=h_2o$
$co+\boxed{o}=co_2$

Important Species

nc_7h_{16}, o_2, $c_7h_{15}\text{-}1/2/3/4$, ho_2, oh, nc_7ket_{24}, nc_7ket_{35}, nc_7ket_{42}, $\cdots$

Generate Skeletal Mechanism

Most-contributing reactions

$\boxed{\mathrm{nc_7h_{16}}}\mathrm{+o_2=}\boxed{\mathrm{c_7h_{15}\text{-}1/2/3/4}}\mathrm{+}\boxed{\mathrm{ho_2}}$

$\mathrm{nc_7h_{16}+oh=c_7h_{15}\text{-}2+ho_2}$
$\mathrm{nc_7h_{16}+oh=c_7h_{15}\text{-}3+ho_2}$
$\boxed{\mathrm{nc_7ket_{24}}}\mathrm{=}\boxed{\mathrm{nc_3h_7cho}}\mathrm{+}\boxed{\mathrm{ch_3coch_2}}\mathrm{+oh}$
$\boxed{\mathrm{nc_7ket_{35}}}\mathrm{=}\boxed{\mathrm{c_2h_5cho}}\mathrm{+}\boxed{\mathrm{c_2h_5coch_2}}\mathrm{+oh}$
$\boxed{\mathrm{nc_7ket_{42}}}\mathrm{=}\boxed{\mathrm{ch_3cho}}\mathrm{+}\boxed{\mathrm{nc_3h_7coch_2}}\mathrm{+oh}$
$\boxed{\mathrm{c_7h_{14}ooh_1\text{-}4}}\mathrm{=}\boxed{\mathrm{c_7h_{14}o_1\text{-}4}}\mathrm{+}\boxed{\mathrm{oh}}$
$\boxed{\mathrm{c_7h_{14}ooh_2\text{-}5}}\mathrm{=}\boxed{\mathrm{c_7h_{14}o_2\text{-}5}}\mathrm{+oh}$
$\boxed{\mathrm{c_7h_{14}ooh_3\text{-}6}}\mathrm{=}\boxed{\mathrm{c_7h_{14}o_2\text{-}5}}\mathrm{+oh}$

$\boxed{\mathrm{ch_2cho}}\mathrm{+o_2=ch_2o+}\boxed{\mathrm{co}}\mathrm{+oh}$
$\boxed{\mathrm{o_2c_2h_4oh}}\mathrm{=oh+2}\boxed{\mathrm{ch_2o}}$

$\boxed{\mathrm{hocho}}\mathrm{+oh=}\boxed{\mathrm{h_2o}}\mathrm{+}\boxed{\mathrm{co_2}}\mathrm{+}\boxed{\mathrm{h}}$
$\mathrm{hocho+h=}\boxed{\mathrm{h_2}}\mathrm{+co_2+h}$
$\mathrm{hocho+oh=h_2o+co_2+h}$
$\mathrm{h+oh=h_2o}$
$\mathrm{co+}\boxed{\mathrm{o}}\mathrm{=co_2}$

Important Species

$\mathrm{nc_7h_{16}}$, $\mathrm{o_2}$, $\mathrm{c_7h_{15}\text{-}1/2/3/4}$, $\mathrm{ho_2}$, oh, $\mathrm{nc_7ket_{24}}$, $\mathrm{nc_7ket_{35}}$, $\mathrm{nc_7ket_{42}}$, $\cdots$

Skeletal Mechanism Generation

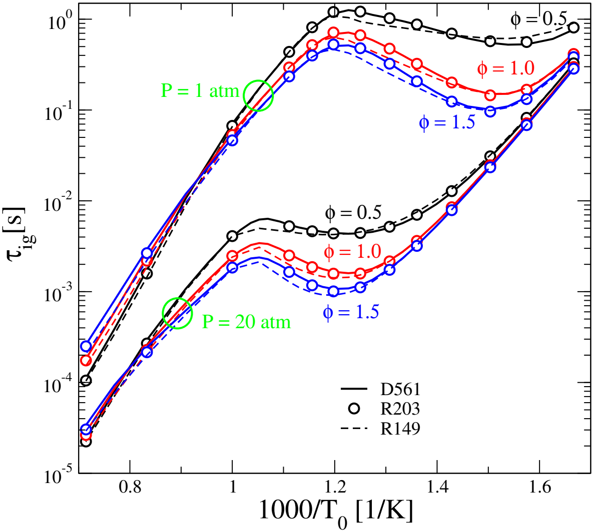
- Eliminate non-important species
- Keep all elementary reactions including important species

Skeletal Mechanism for *n*-heptane/air kinetics

- Detailed Mechanism (D561): $n_s = 561$, $n_r = 2539$
- Sampled points took from autoignition in adiabatic constant pressure reactor
  - $650 \leq T_0 \leq 1400$ K
  - $1 \leq P \leq 20$ atm
  - $0.5 \leq \phi \leq 1.5$
- $\varepsilon = 0.2\% \longrightarrow n_s = 203, n_r = 879$ (R203)
- $\varepsilon = 0.6\% \longrightarrow n_s = 149, n_r = 669$ (R149)

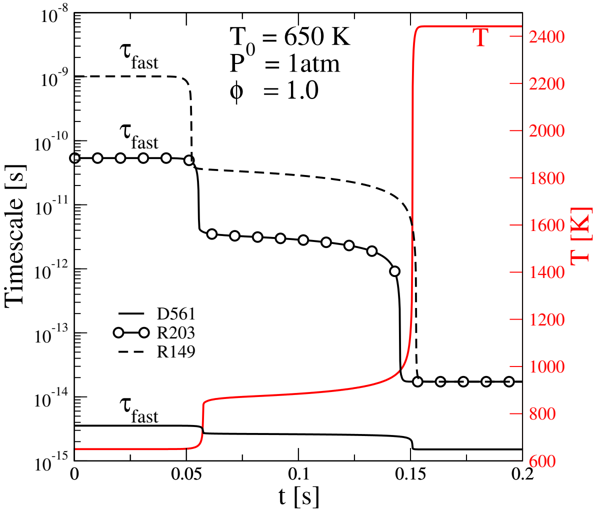
Kooshkbaghi, M., et al., (2014). *Combust. Flame, 161(6)*, 1507-1515.

Validation : Ignition Delay



Kooshkbaghi, M., et al., (2014). *Combust. Flame, 161(6)*, 1507-1515.

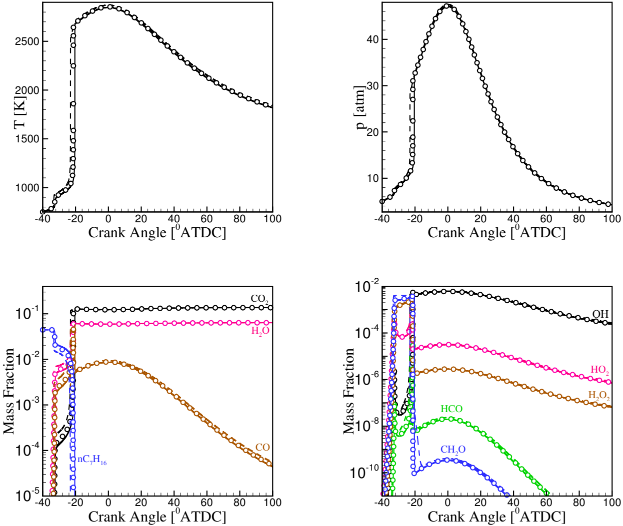
Stiffness



Kooshkbaghi, M., et al., (2014). *Combust. Flame, 161(6)*, 1507-1515.

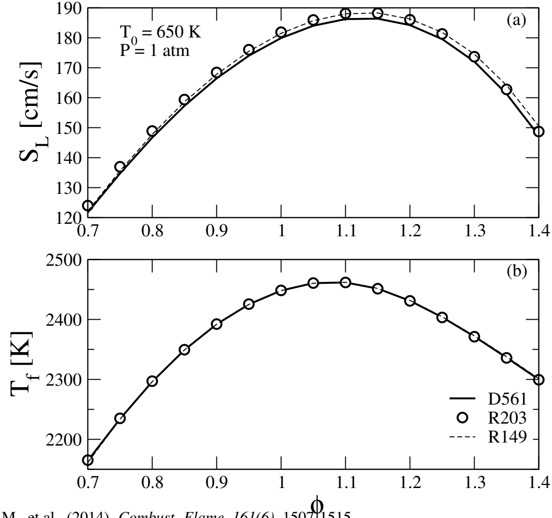
Validation : Single-Zone Engine Model

$T_{inlet} = 650$ K, $P_{inlet} = 5$ atm, $\phi = 0.8$ at $-40\ ^{o}$ATDC, $\omega = 700$ rpm



Validation : Laminar Premixed Flame

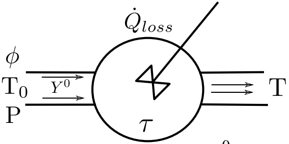
$T_u = 650$ K, $P = 1$ atm



Kooshkbaghi, M., et al., (2014). *Combust. Flame, 161(6)*, 1507–1515.

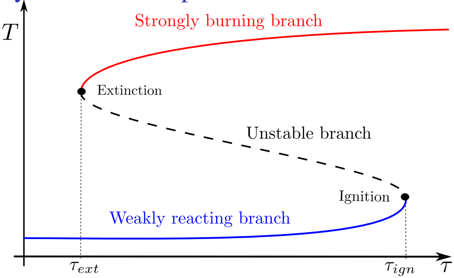
IV. *n*-heptane/air complex dynamics

PSR setup and hysteresis of temperature



$$\frac{dY_k}{dt} = \frac{W_k \dot{\omega}}{\rho} + \frac{Y_k^0 - Y_k}{\tau}$$

$$\frac{dT}{dt} = -\frac{\sum_{i=1}^{n_s} W_i \dot{\omega}_i h_i}{\rho c_p} + \frac{\sum_{i=1}^{n_s} Y_i^0 (h_i^0 - h_i)}{c_p \tau} - \frac{\dot{Q}_{loss}}{\rho c_p}$$



Typical S-shaped bifurcation diagram of a PSR

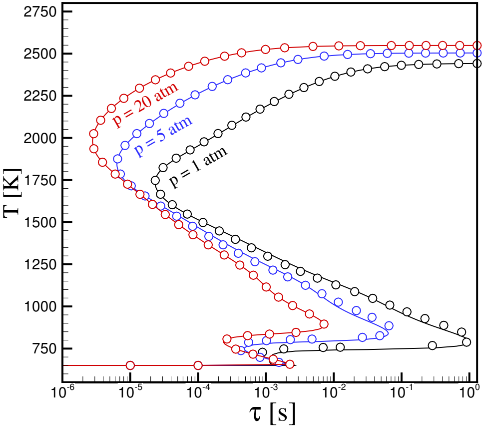
Parameters

τ: Residence Time
p: Reactor Pressure
ϕ: Inlet Mixture
T_0: Inlet Temperature
$\dot{Q}_{loss}$: Heat loss per unit volume

Numerical tool

AUTO-07p: Continuation and Bifurcation Software for ODEs + CHEMKIN III: Chemical kinetics data

Validation Of Skeletal Mechanism



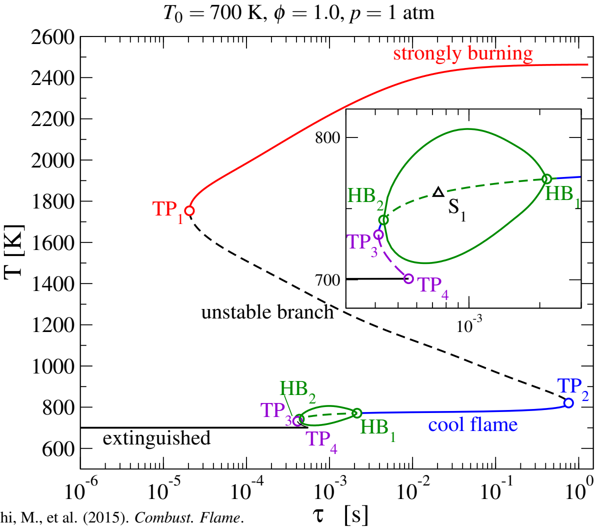
Dependence of reactor temperature on residence time of adiabatic PSR

$T_0 = 650$ K, $\phi = 1.0$

D561 (solid lines) and R149 (open circles)

One parameter continuation

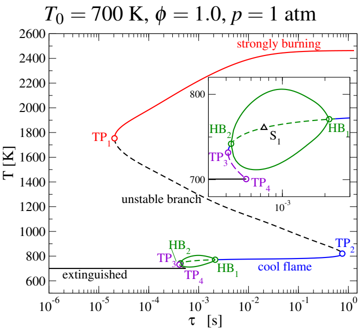
Reactor Temperature vs Residence Time

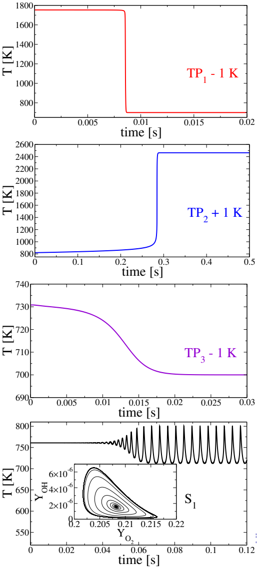


Kooshkbaghi, M., et al. (2015). *Combust. Flame*.

One parameter continuation

Reactor Temperature vs Residence Time

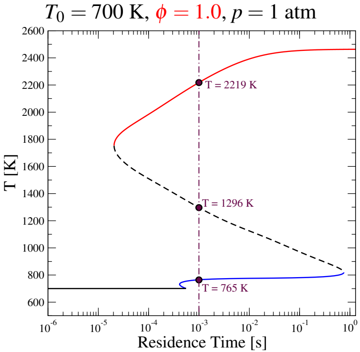


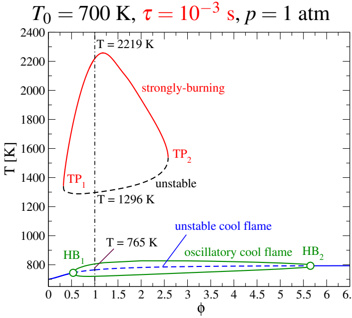


Kooshkbaghi, M., et al. (2015). *Combust. Flame*.

One parameter continuation

Reactor Temperature vs Equivalence ratio

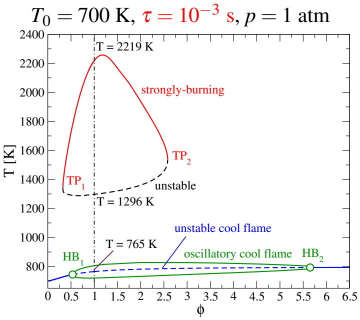

$T_0 = 700$ K, $\phi = 1.0$, $p = 1$ atm

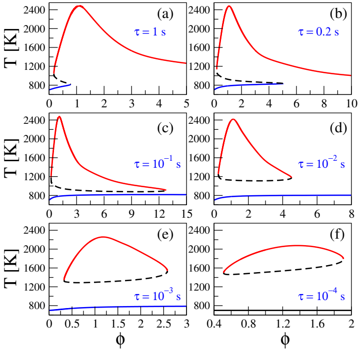

$T_0 = 700$ K, $\tau = 10^{-3}$ s, $p = 1$ atm

For fixed residence time, the change of reactor temperature respect to the inlet mixture composition.

One parameter continuation

Reactor Temperature vs Equivalence ratio

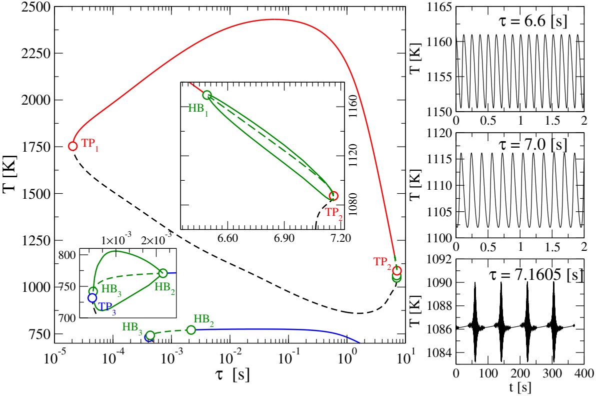




For fixed residence time, the change of reactor temperature respect to the inlet mixture composition.

One parameter continuation

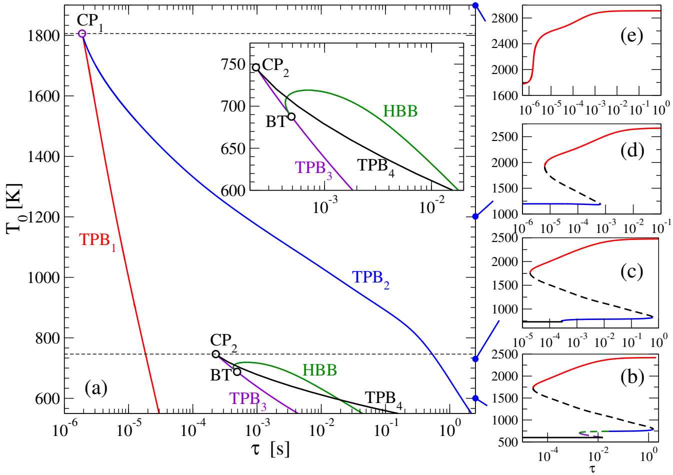
Reactor Temperature for non-adiabtic reactors



Dependence of reactor temperature on residence time for non-adiabatic PSR
$p = 1$ atm, $T_0 = 700$ K, $\phi = 1$ and $\dot{Q}_{loss} = 0.1 kJ/(s \times m^3)$

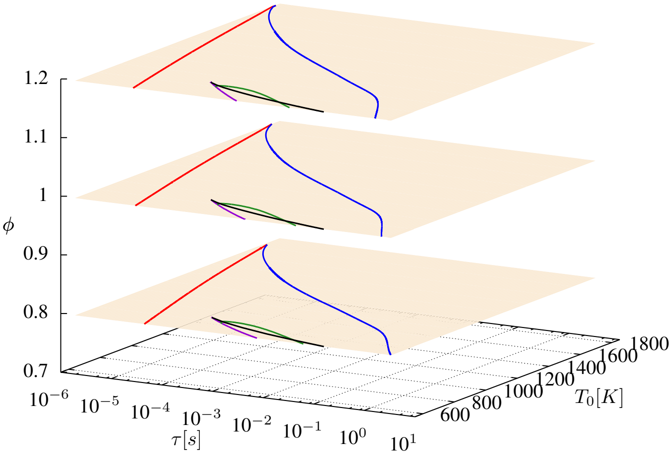
Multi-parameter continuation

Continuation in $(T_0 - \tau)$ parameters

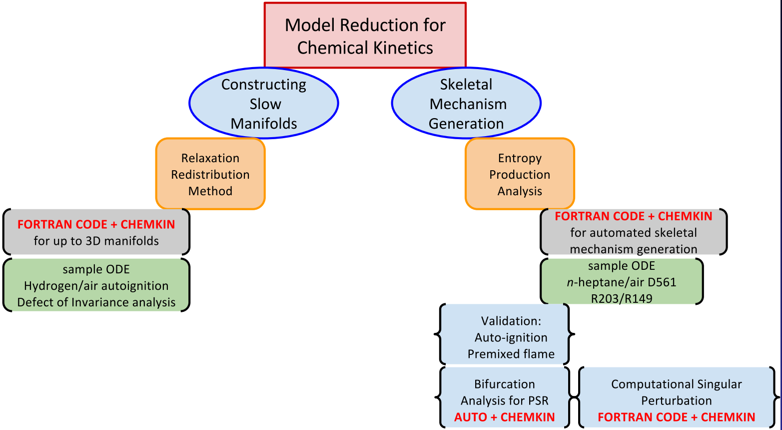


Multi-parameter continuation

Continuation in $(T_0 - \tau - \phi)$ parameters



Summary



Model Reduction for Chemical Kinetics

Constructing Slow Manifolds

Relaxation Redistribution Method

FORTRAN CODE + CHEMKIN
for up to 3D manifolds

sample ODE
Hydrogen/air autoignition
Defect of Invariance analysis

Skeletal Mechanism Generation

Entropy Production Analysis

FORTRAN CODE + CHEMKIN
for automated skeletal mechanism generation

sample ODE
n-heptane/air D561
R203/R149

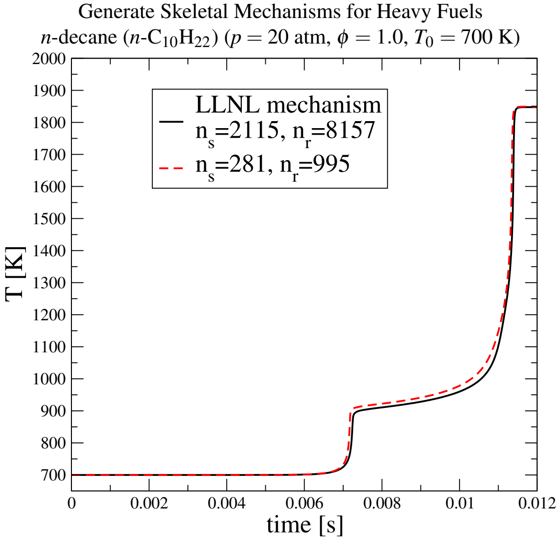
Validation:
Auto-ignition
Premixed flame

Bifurcation Analysis for PSR
AUTO + CHEMKIN

Computational Singular Perturbation
FORTRAN CODE + CHEMKIN

Directions for future work

- Entropy Production Analysis

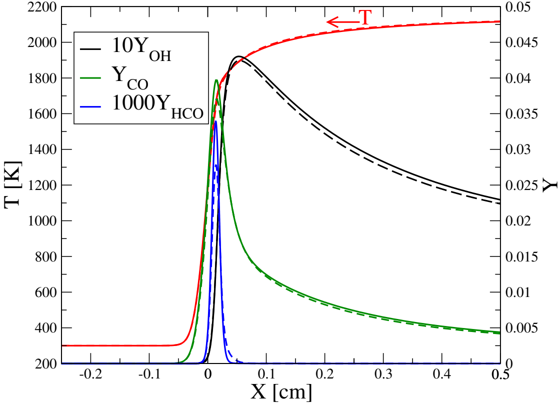


Directions for future work

- Entropy Production Analysis

Direct Numerical Simulations using skeletal mechanisms

CH_4/air premixed flame ($p = 1$ atm, $\phi = 0.9$, $T_0 = 300$ K, $\delta_f = \frac{T_f - T_0}{max|\frac{dT}{dx}|}$)



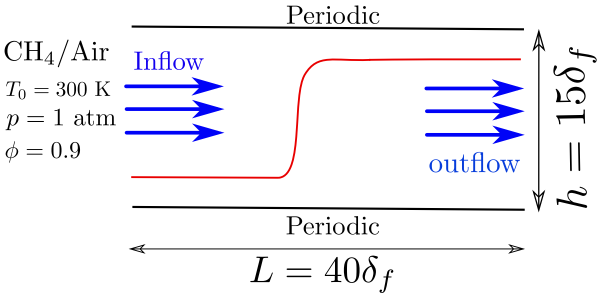
Detailed D35 (solid lines), Skeletal R20 (dashed lines)

Directions for future work

- Entropy Production Analysis

Direct Numerical Simulations using skeletal mechanisms

CH_4/air premixed flame ($p = 1$ atm, $\phi = 0.9$, $T_0 = 300$ K, $\delta_f = \frac{T_f - T_0}{max|\frac{dT}{dx}|}$)



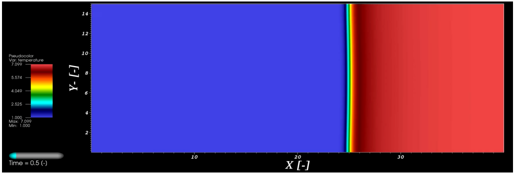
Directions for future work

- Entropy Production Analysis

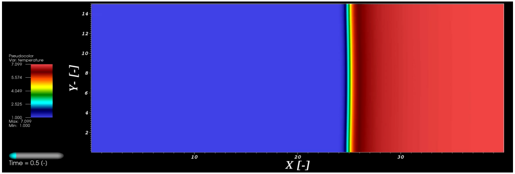
Direct Numerical Simulations using skeletal mechanisms

CH_4/air premixed flame ($p = 1$ atm, $\phi = 0.9$, $T_0 = 300$ K, $\delta_f = \frac{T_f - T_0}{max|\frac{dT}{dx}|}$)

Temperature contours
Detailed (D35)



Reduced (R20)



Publications

Journal Publications

1. **Kooshkbaghi, M.**, Frouzakis, C. E., Chiavazzo, E., Boulouchos, K., & Karlin, I. V. (2014). The global relaxation redistribution method for reduction of combustion kinetics. *J. Chem. Phys. 141(4)*, 044102.
2. **Kooshkbaghi, M.**, Frouzakis, C. E., Boulouchos, K., & Karlin, I. V. (2014). Entropy production analysis for mechanism reduction. *Combust. Flame, 161(6)*, 1507-1515.
3. Karlin, I. V., Chikatamarla, S. S., & **Kooshkbaghi, M.** (2014). Non-perturbative hydrodynamic limits: A case study. *Physica A, 403*, 189-194.
4. **Kooshkbaghi, M.**, Frouzakis, C. E., Boulouchos, K., & Karlin, I. V. (2015). n-Heptane/air combustion in perfectly stirred reactors: Dynamics, bifurcations and dominant reactions at critical conditions. *Combust. Flame.*
5. **Kooshkbaghi, M.**, Frouzakis, C. E., Boulouchos, K., & Karlin, I. V. (2015). Spectral Quasi Equilibrium Manifold for Chemical Kinetics. *In preparation for J. Chem. Phys.*

Conferences

1. **Kooshkbaghi, M.**, Frouzakis, C. E., Chiavazzo, E., Karlin, I. V., & Boulouchos, K. (2013). IWMRRF, San Francisco, California, USA.
2. **Kooshkbaghi, M.**, Boulouchos, K., Frouzakis, C. E., Karlin, I. V., & Chiavazzo, E. (2013). IEA, 36th TLM, Stavanger, Norway.

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