Skeletal Reaction Models Based on Principal Component Analysis: Application Ignition, Propagation and Extinction Phenomena

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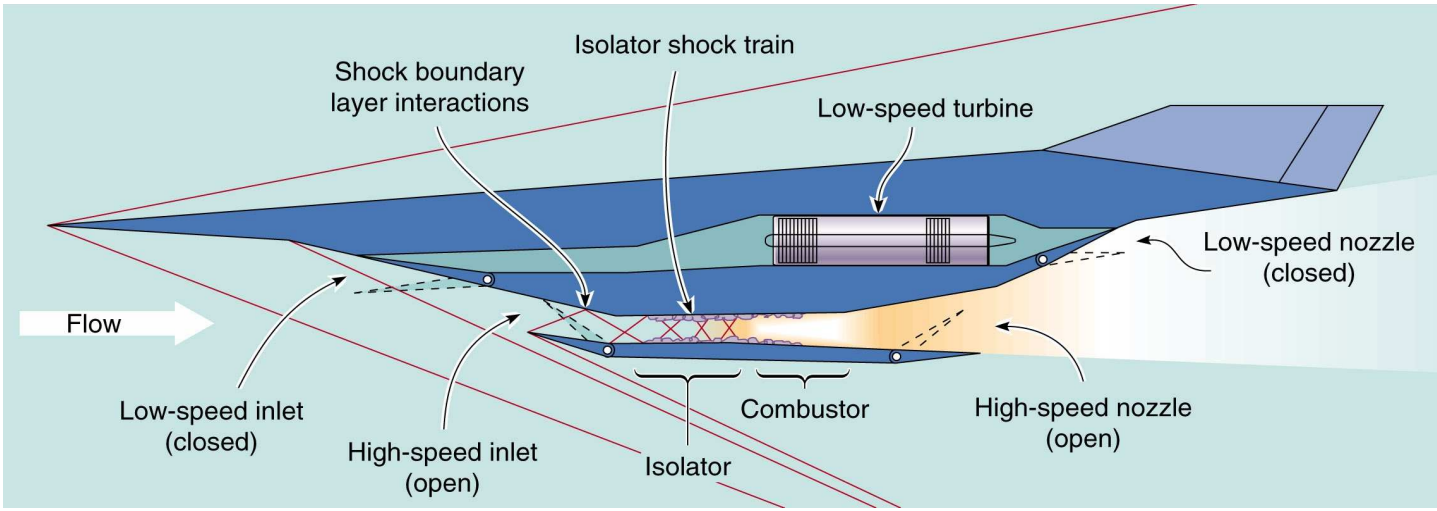
Motivation

- Skeletal and reduced reaction models for hypersonic propulsion applications

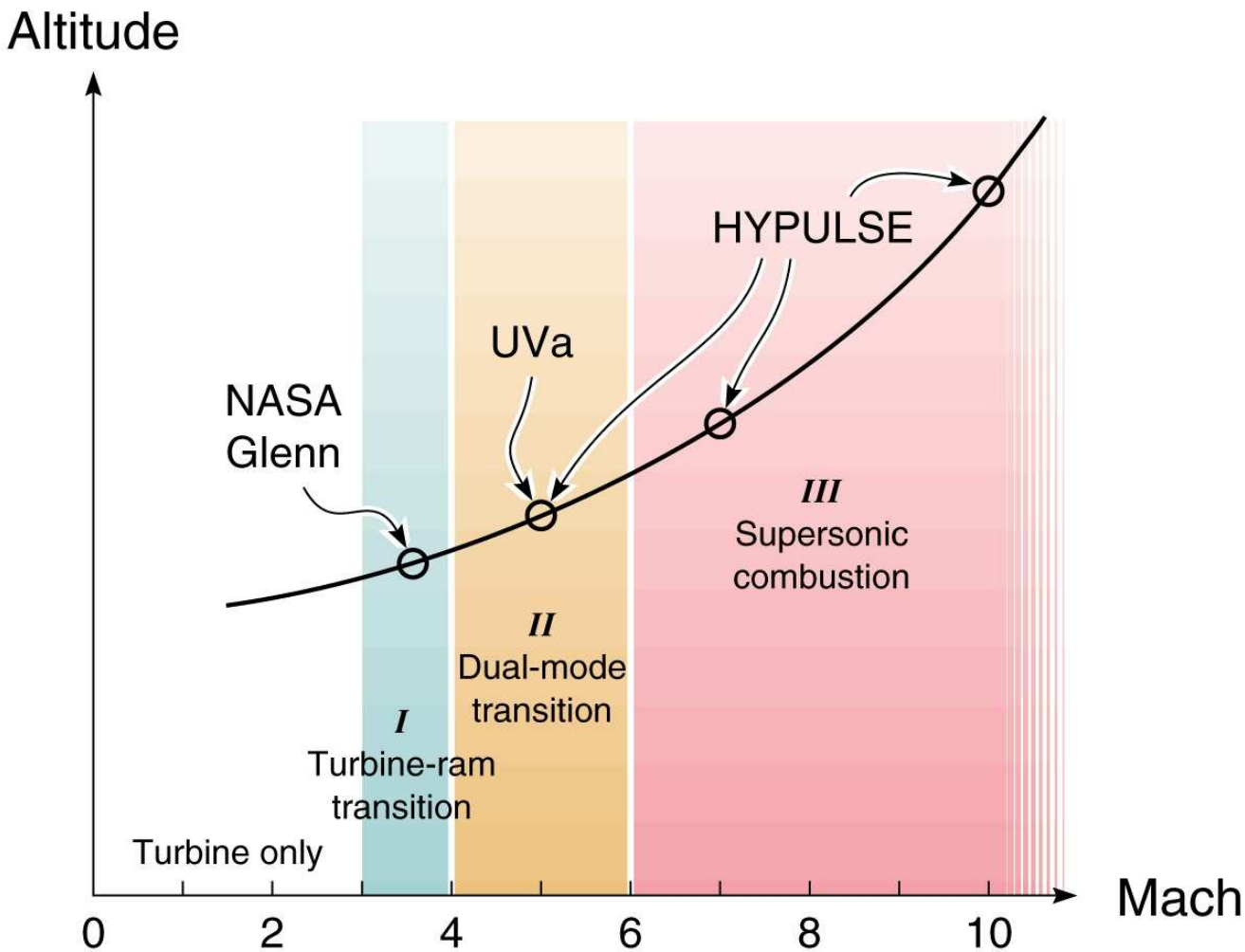


FOCUS:

- C1-C4 skeletal and reduced reaction models, eg. hydrogen, methane, ethylene, propene, 1-butene, ...

Motivation

- Skeletal and reduced reaction models for hypersonic propulsion applications



Principal Component Analysis with Sensitivity (PCAS)

- Starting point of PCAS is the construction of response function (Vajda, Valko, and Turanyi (1985)):

$$\boxed{Q(\mathbf{P}) = \sum_{j=1}^{q} \sum_{i=1}^{m} \left[\frac{f_i(x_j, \mathbf{P}) - f_i(x_j, \mathbf{P^0})}{f_i(x_j, \mathbf{P^0})} \right]^2}$$

where $\mathbf{P}$, $\mathbf{P^0}$ are unperturbed and perturbed parameters ($k = 1, ..., p$); f_i a set of target functions ($i = 1, ..., m$); x_j collection of analysis points ($j = 1, ..., q$).

- Around $\mathbf{P^0}$, the response function can be approximated as:

$$Q(\mathbf{P}) \approx q(\mathbf{P}) = (\Delta\mathbf{P})^T \, \mathbf{S}^T\mathbf{S}(\Delta\mathbf{P}) = (\Delta\mathbf{P})^T \, \mathbf{U}^T\Lambda\mathbf{U}(\Delta\mathbf{P}) = \boxed{\sum_{k=1}^{p} \lambda_k (\Delta\Psi_k)^2}$$

where $\Delta\mathbf{P} = \mathbf{P} - \mathbf{P^0}$; $\mathbf{S}$ collection of sensitivity matrices; λ_k eigenvalues; $\mathbf{U}$ normalized eigenvectors; $\boldsymbol{\Delta\Psi} = \mathbf{U}^T\mathbf{P}$ principal components.

Combined Response Function for Ignition, Propagation, and Extinction

- Can combine sensitivity matrices for any phenomena of interest and construct a combined response function:

$$
\begin{aligned}
Q^C(\mathbf{P}) \quad = \quad & \left\{ \sum_{j=1}^{l} \sum_{i=1}^{m} \left[\frac{f_i(x_j, \mathbf{P}) - f_i(x_j, \mathbf{P^0})}{f_i(x_j, \mathbf{P^0})} \right]^2 \right\}_{\text{phen } 1} \\
+ \quad & \left\{ \sum_{j=1}^{l} \sum_{i=1}^{m} \left[\frac{g_i(x_j, \mathbf{P}) - g_i(x_j, \mathbf{P^0})}{g_i(x_j, \mathbf{P^0})} \right]^2 \right\}_{\text{phen } 2} \\
+ \quad & \ldots + \left\{ \sum_{j=1}^{l} \sum_{i=1}^{m} \left[\frac{h_i(x_j, \mathbf{P}) - h_i(x_j, \mathbf{P^0})}{h_i(x_j, \mathbf{P^0})} \right]^2 \right\}_{\text{phen } \alpha} ,
\end{aligned}
$$

where target functions $f_i, g_i, h_i, \ldots$ can be any phenomenon α.

Selection of Target Functions or Sensitivities

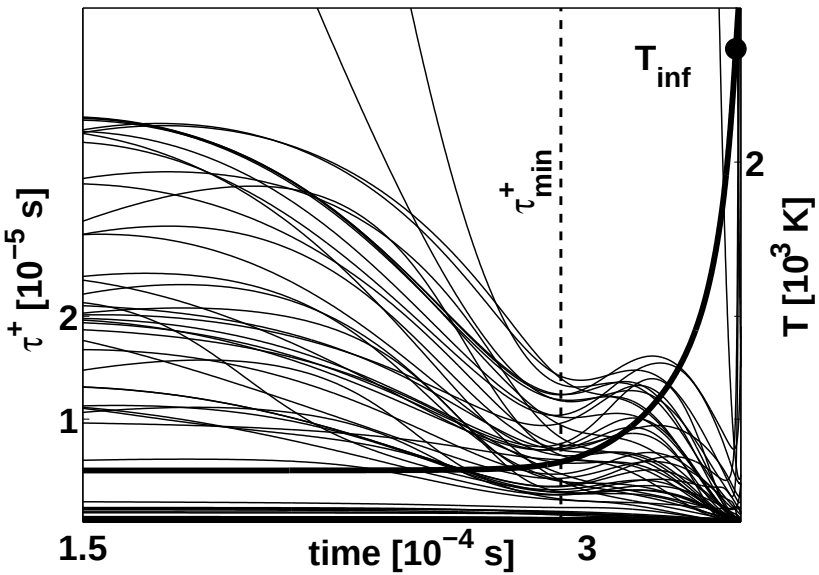
- Structural features, eg. $Y_i, T, \omega_i, \dot{q}, \ldots$
- Global features, eg. ignition delay, burning velocity, extinction limits, ...
- In this work, sensitivities of $T, \dot{q}, \tau, S_L^0, a_{ext}$ have been included.
- In particular, $\partial \dot{q} / \partial k_k$ is evaluated from

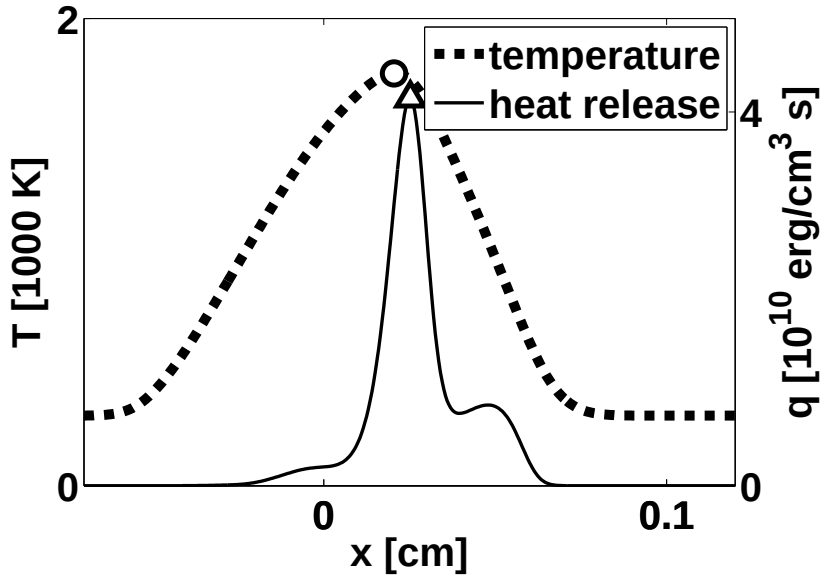
$$\frac{\partial \dot{q}}{\partial k_k} = \frac{\partial T}{\partial k_k} \sum_{i=1}^{N_{sp}} c_{p_i} \dot{\omega}_i + \frac{\partial T}{\partial k_k} \sum_{i=1}^{N_{sp}} h_i \left[\sum_{k=1}^{r} \left(\frac{\beta_k}{T} - \frac{E_k}{R^o T^2} \right) \nu_{ik} \hat{\omega}_k \right] +$$

$$+ \boxed{\rho \sum_{i=1}^{N_{sp}} h_i \left[\sum_{l=1}^{N_{sp}} \left(\frac{1}{W_l c_l} \frac{\partial Y_l}{\partial k_k} \sum_{k=1}^{r} \nu_{ik} \nu_{lk}^{'} \hat{\omega}_k \right) \right]} + \sum_{i=1}^{N_{sp}} h_i \nu_{ik} \prod_{l=1}^{N_{sp}} c_l^{\nu_{lk}^{'}}$$

Selection of Temporal or Spatial Location for Sensitivity Analyis

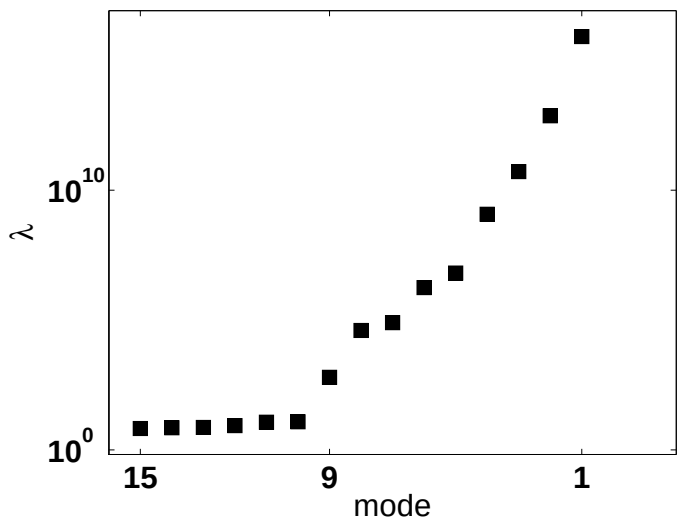
- To minimize the size of combined sensitivity matrix, optimum temporal (in homogeneous ignition) or spatial (in pre-
mixed and non-premixed flames) locations were selected for sensitivity analysis.

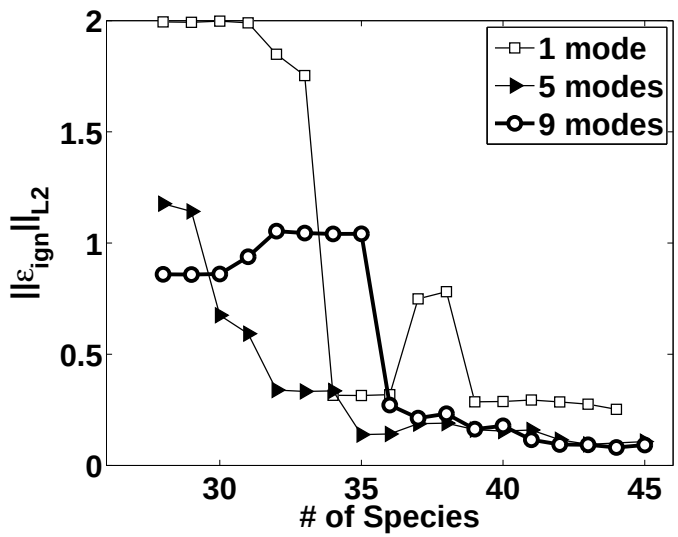




Selection of Number of Modes

- Number of eigenvalues and eigenvectors to be retained in PCAS analysis is somewhat uncertain!
- For ignition and for 9 distinct cases of initial conditions:



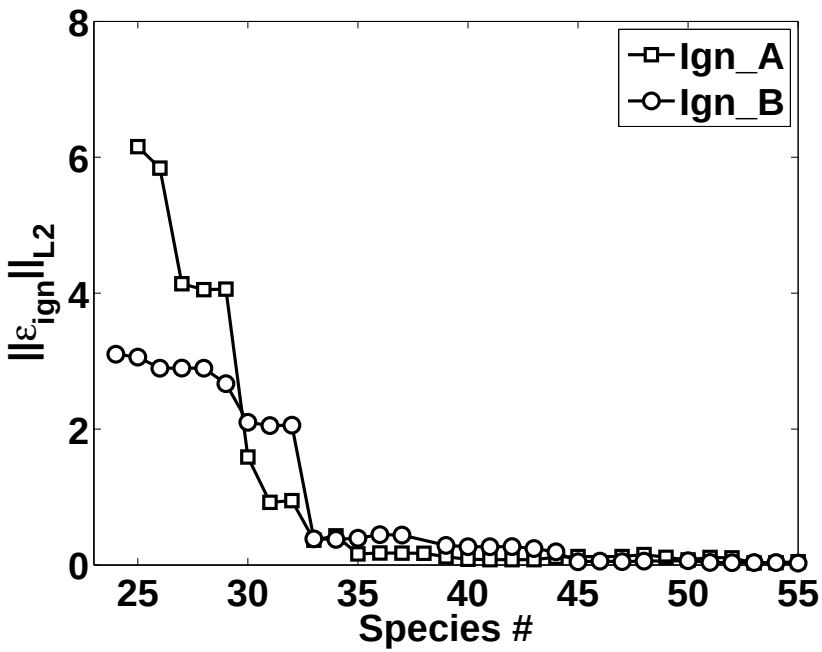


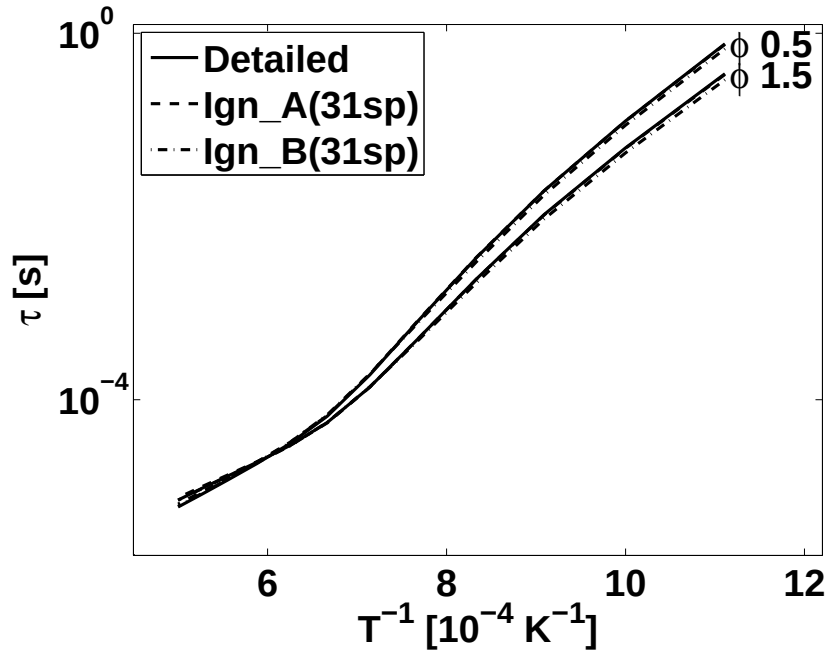
- Error measure is integrated over the range of T_0 and ϕ:

$$||\epsilon_{ign}||_{L_2} = [\int_{\phi_a}^{\phi_b} \int_{T_a}^{T_b} ((\tau_{ign,skel} - \tau_{ign,det})/\tau_{ign,det}))^2 \mathrm{d}T \mathrm{d}\phi]^{1/2}$$

Skeletal Models Based on Ignition Analysis Only

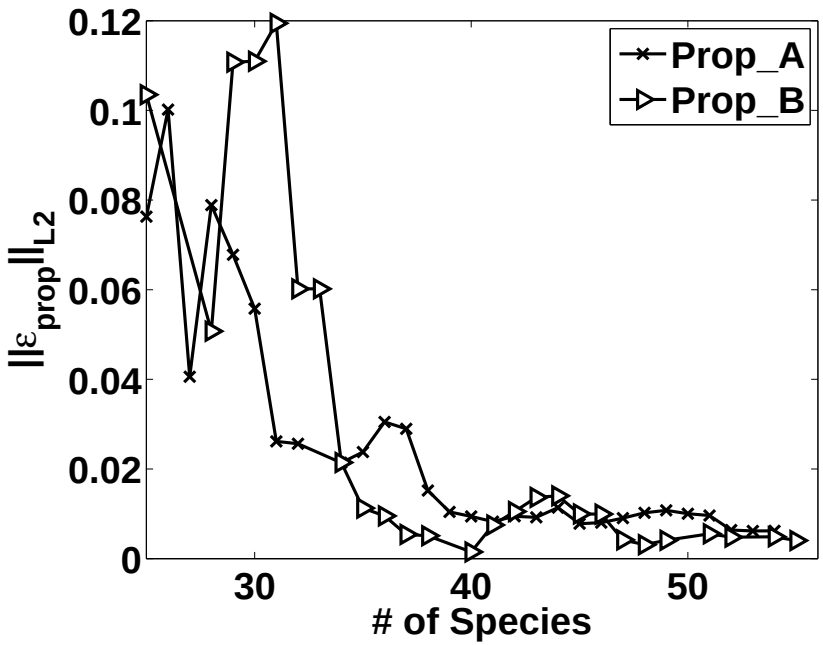
- USC Mech II(opt) (Sheen et al., 2009) with 111 species in 784 reactions.
- Application to ignition of ethylene-air mixtures at p =1 atm.

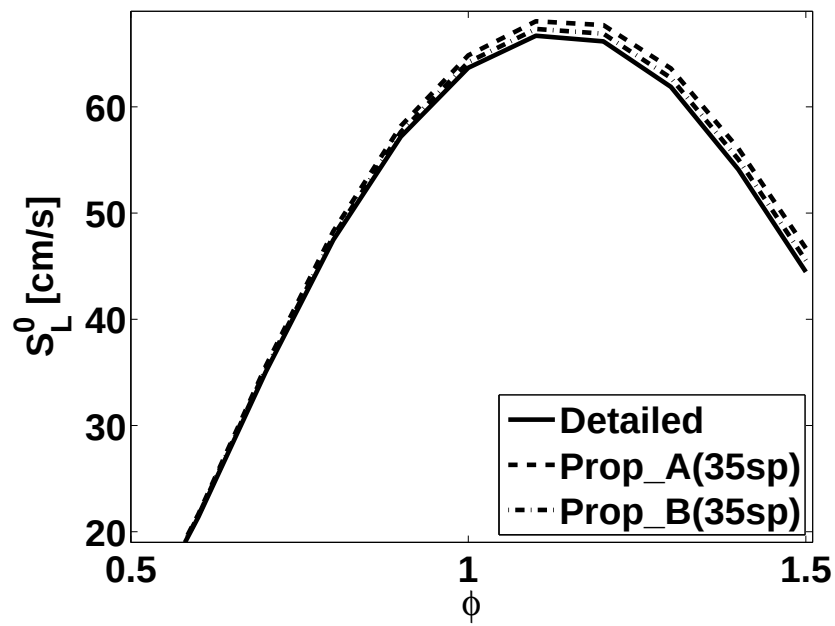




Skeletal Models Based on Flame Propagation Analysis Only

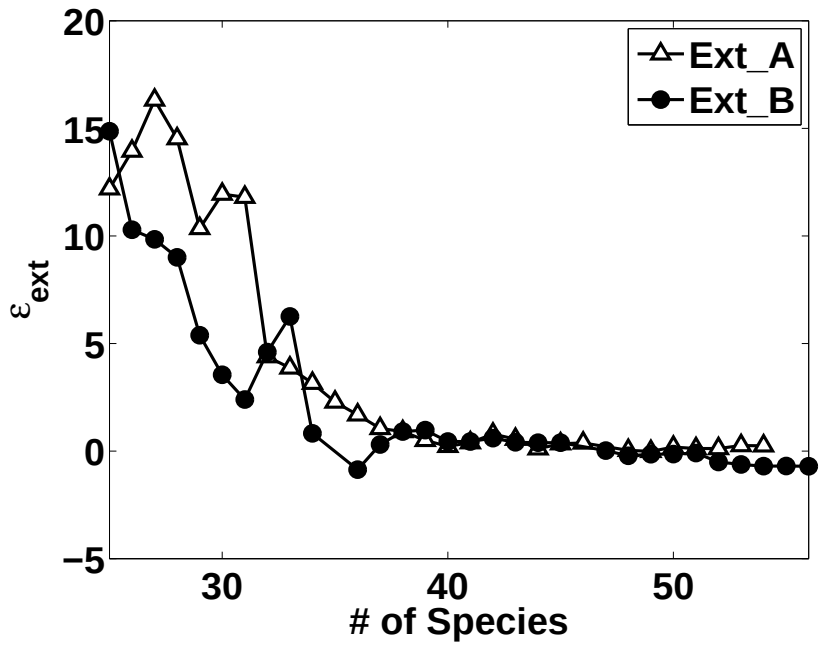
- Ethylene-air mixtures at p=1.0atm and T_0=300 K.

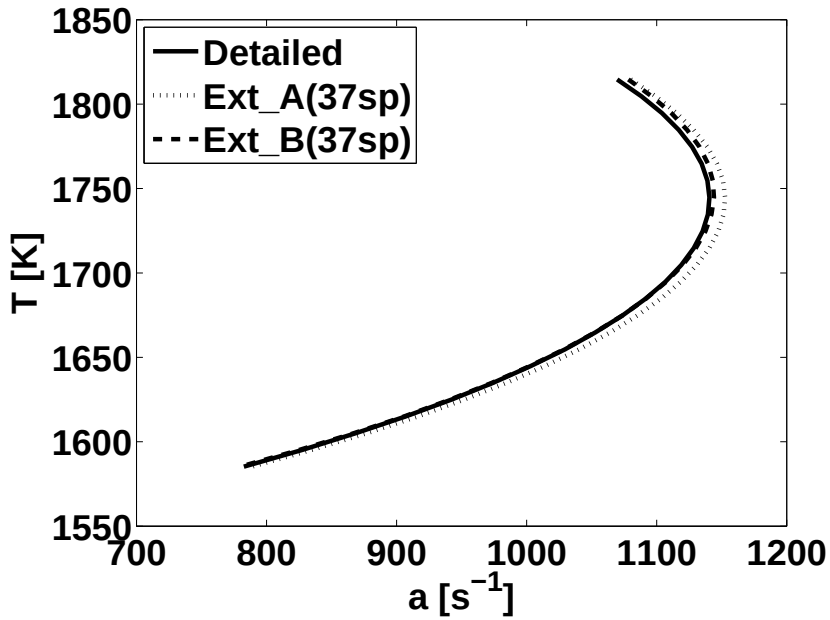




Skeletal Models Based on Flame Extinction Only

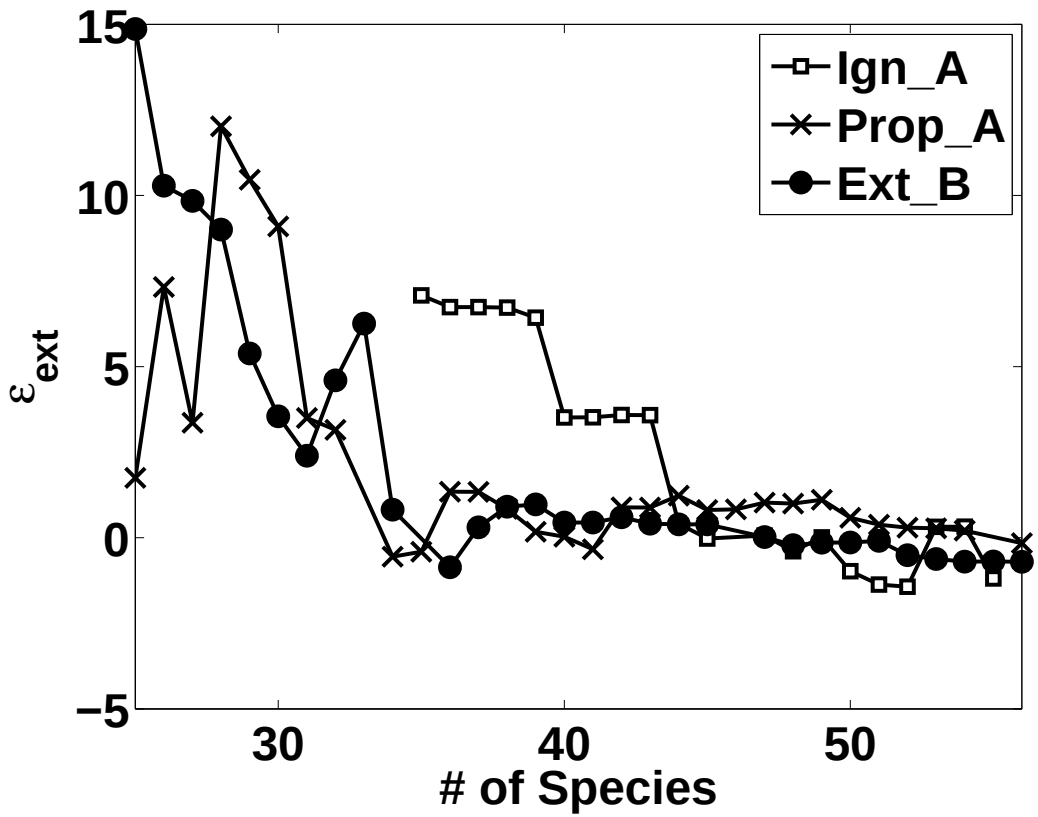
- Non-premixed ethylene and air, at p=1.0atm, T_0=300 K.





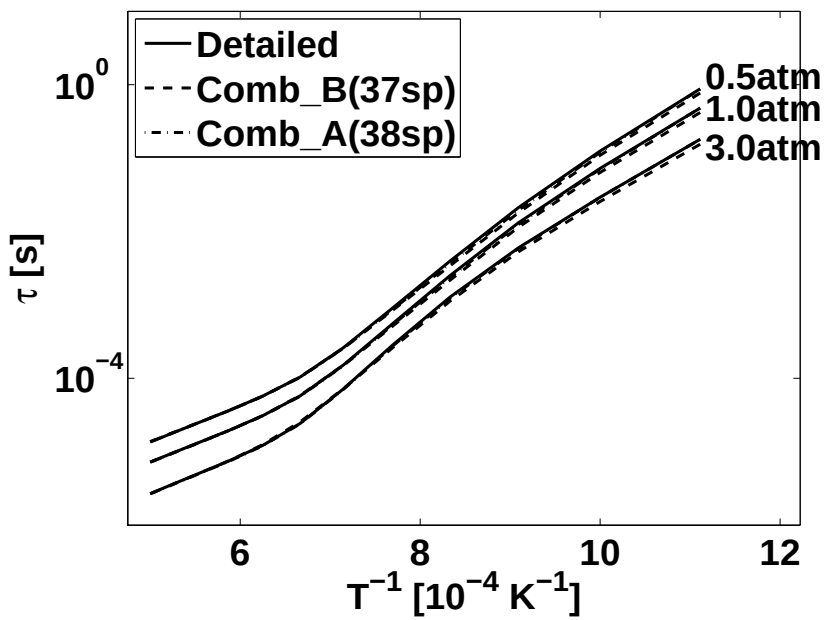
Can Extinction limits be Predicted by Ignition and Propagation Analysis?

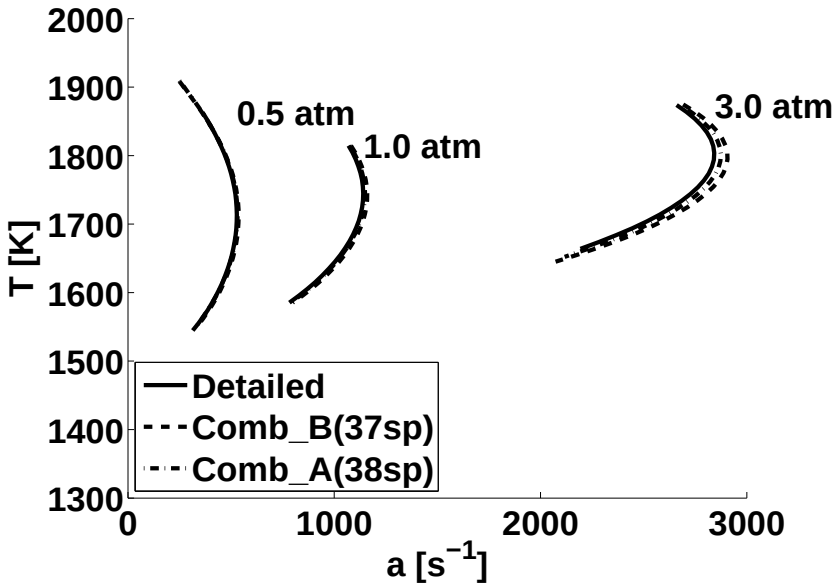
- Comparison of the extinction limit error predicted from models based on ignition, propagation, and extinction analyses.



Combined Skeletal Models

- From combined analysis, two skeletal models have been recommended for ethylene-air mixtures (37 and 38 species) – see Esposito and Chelliah, *Combustion and Flame*, in print.

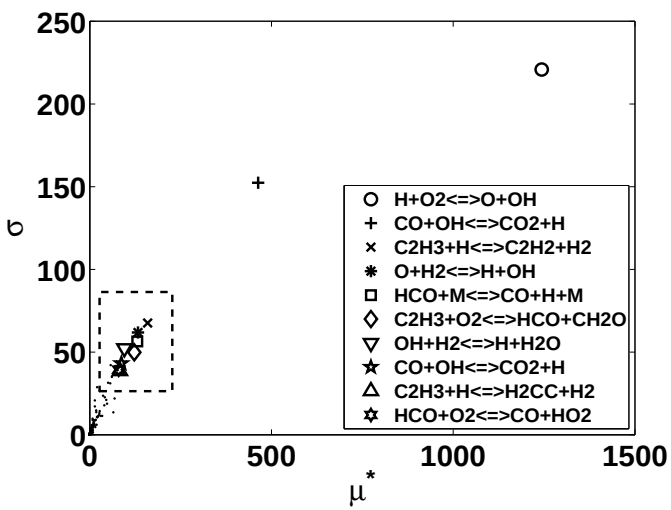




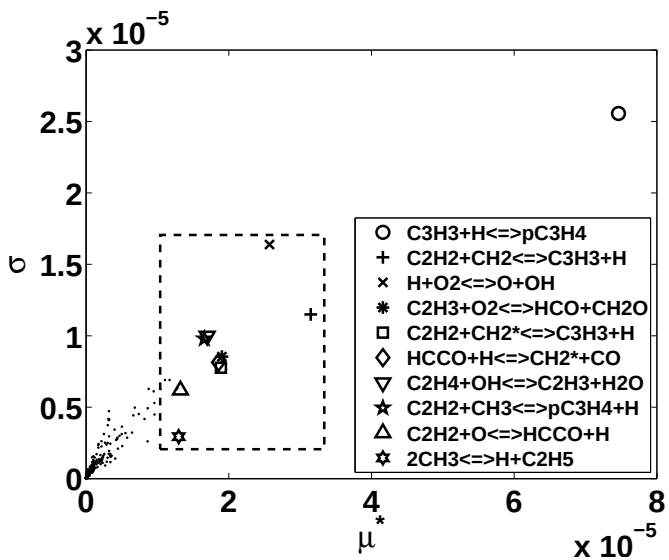
- QSSA Reduction Approach has been applied to derive a new 20-step reduced reaction model [20 species + 3 species (element conservation)]

Reaction Rate Uncertainty Analysis and Error Propagation

- Monte Carlo simulations have been performed to understand the impact of rate constant uncertainties on flame extinction predictions
— full MC simulations require 2^p calculations, where $p = 784$! Impossible!
— used screening methods, i.e. local sensitivity and Morris method ($r \times (p+1) \equiv 15700$ simulations), to identify top 14 reactions
- Morris method results:



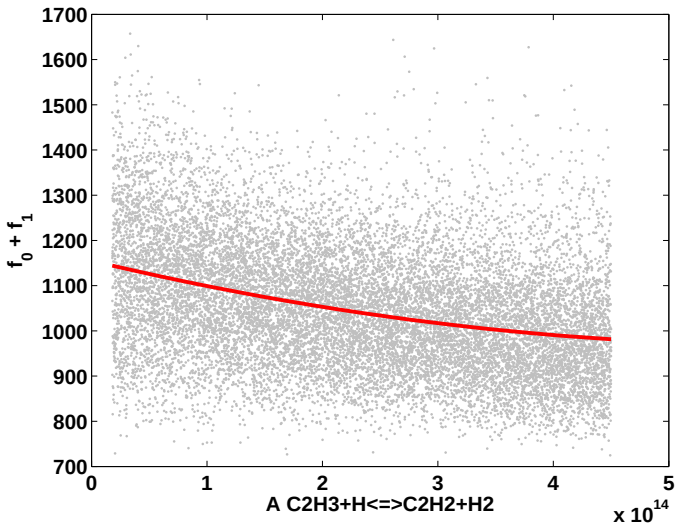
sensitive reactions for extinction



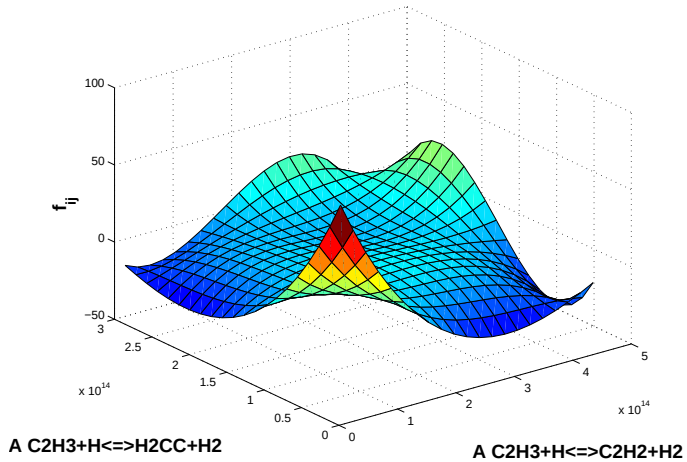
sensitive reactions for C3H3 formation

Reaction Rate Uncertainty Analysis and Error Propagation

- full MC simulation of 14 reactions requires $3 \times (2^{14}) = 49152$ flame calculations (about 2000 days!) - used distributed computing!
- From MC simulation of 14 rate constant uncertainties on flame extinction, can identify (i) non-linear contributions and (ii) error propagation (forward and backward)



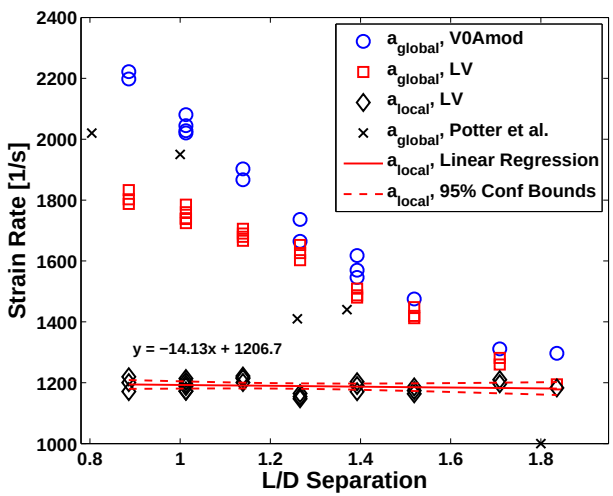
First order term



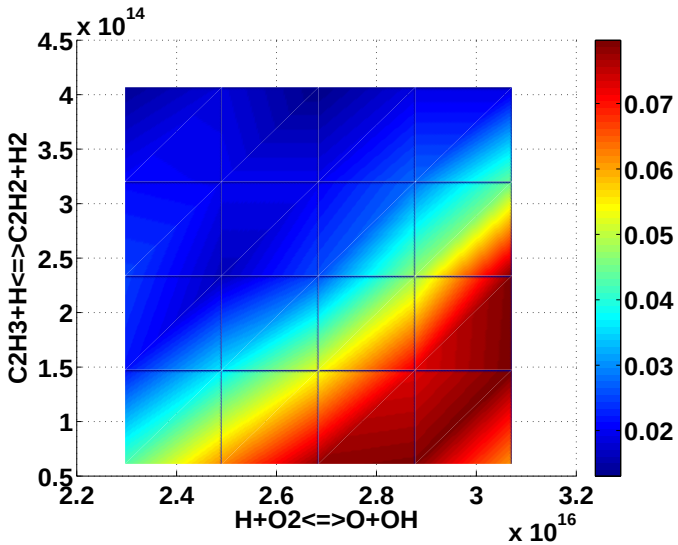
Second-order term

Reaction Rate Uncertainty Analysis and Error Propagation

- From MC simulation of 14 rate constant uncertainties on flame extinction, can identify (i) non-linear contributions and (ii) error propagation (forward and backward)



UVa ethylene-air extinction data



reduced uncertainty range

Reaction Rate Uncertainty Analysis and Error Propagation

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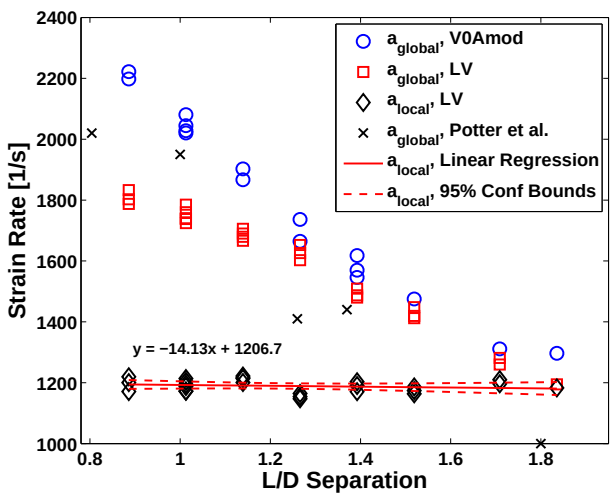

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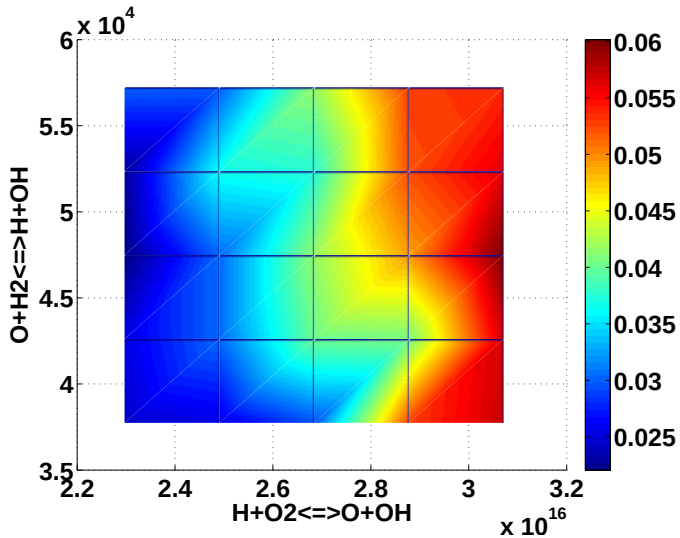

reduced uncertainty range

- Used an uncertainty factor of 1.2 for H+O2=OH+O and MC results show that high end is most probable???

Conclusions

- PCA based methods can be used efficiently to derive skeletal reaction models
- Prediction of flame extinction is often the limiting factor for further reduction of the size of skeletal reaction models
- Previously reported QSSA approach has been utilized to obtain a 20 step reduced reaction model for ethylene
- High-performance computing facilities have been utilized to explore first-order and second-order effects of rate constants controlling flame extinction, formation of soot precursors, etc.

$\Rightarrow$ this approach can also be used to narrow the uncertainty factor knowing accurate uncertainty bounds of experimental data

- Acknowledgments:
  - Hai Wang and David Sheen for sharing kinetic models
  - AFOSR/NASA National Center for Hypersonic Combined-Cycle Propulsion