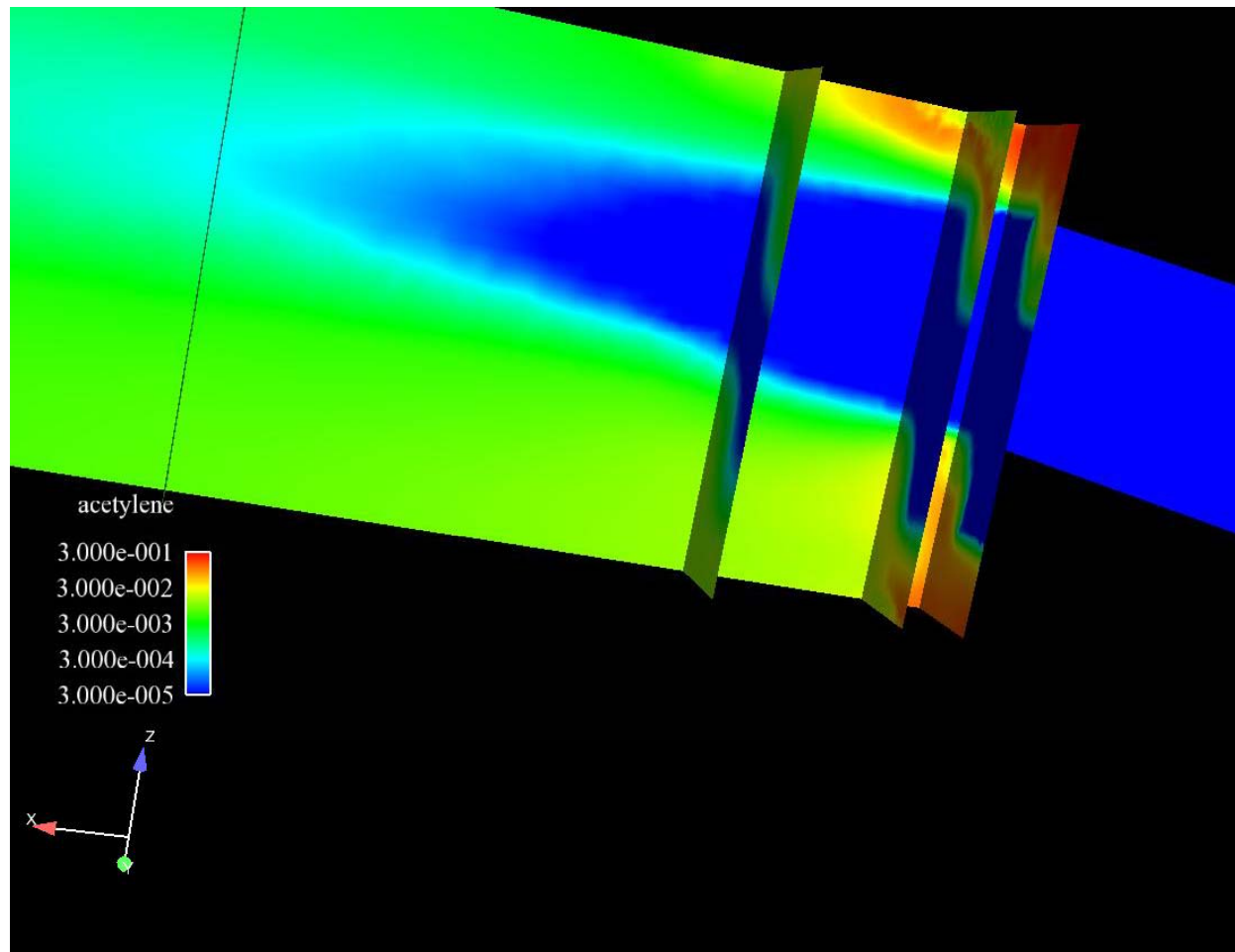


# *Roadrunner Kinetics*

## Custom Reduced Mechanisms for CFD

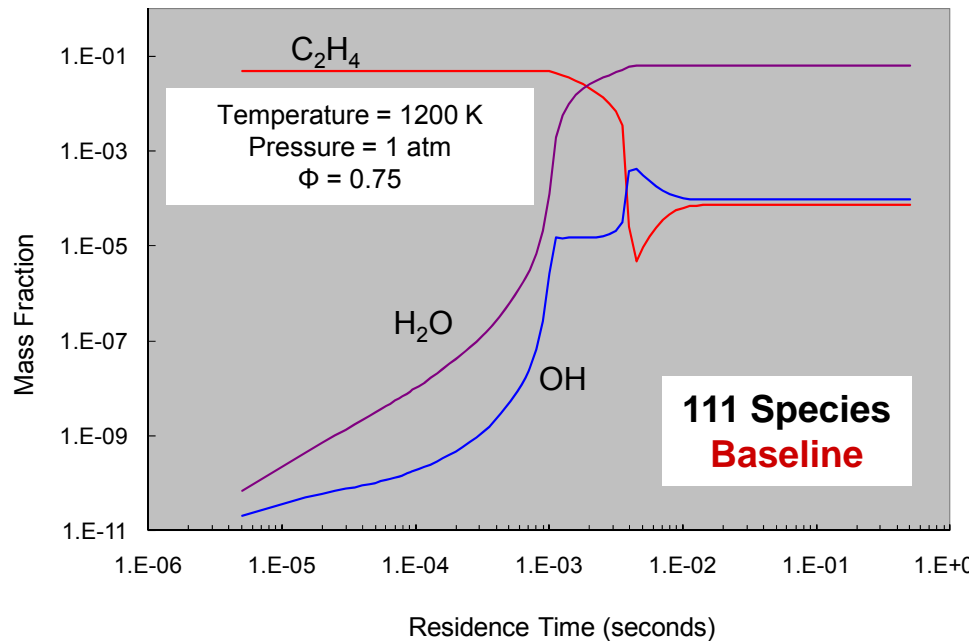


# Our Reduced Kinetic Models Have Superior Accuracy

## Full Mechanism

Ethylene combustion

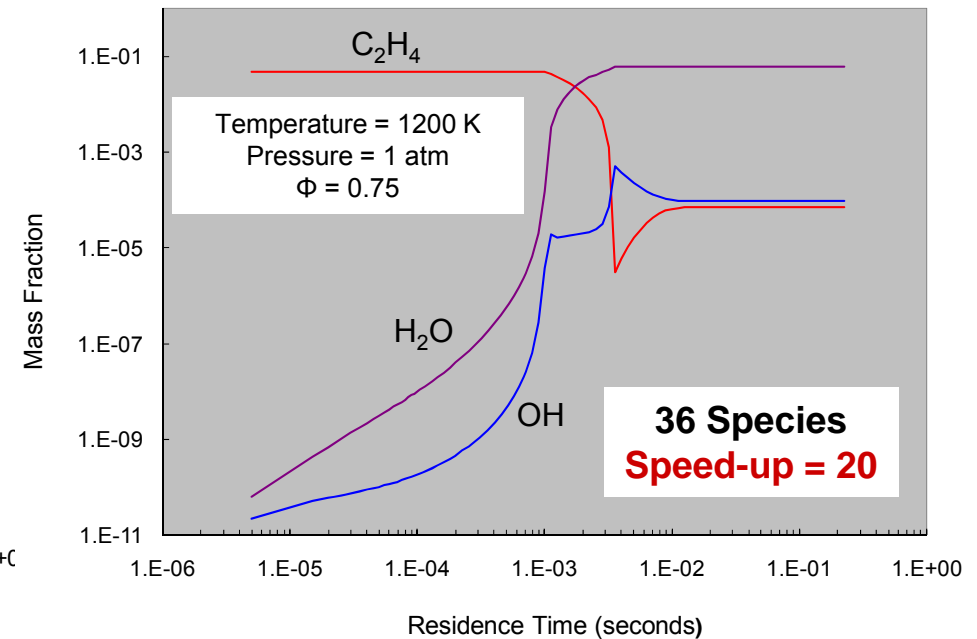
111 species; 781 reactions



## Reaction Systems Reduced Mechanism I

36 species; 216 reactions

- Factor of 20 speedup!
- Accurately predicts the two-stage ignition process.

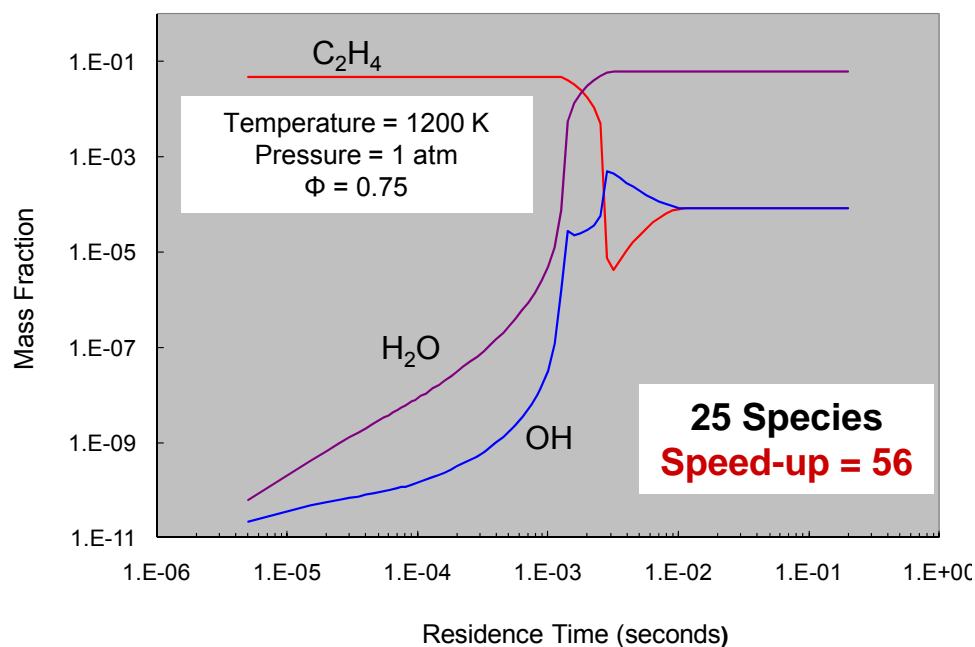


# Mechanism Suite Will Provide Desired Balance of Accuracy and Speed

## Reduced Mechanism II

25 species; 107 reactions

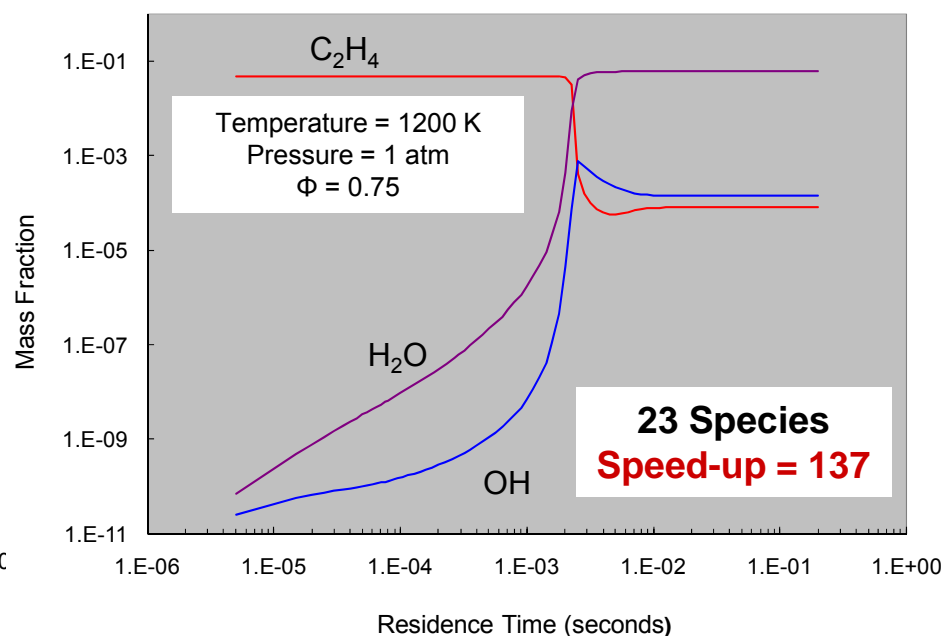
- Factor of 56 speedup!
- Still captures the two-stage ignition process.



## Reduced Mechanism III

23 species; 84 reactions

- Factor of 137 speedup!
- Numerically more stable
- Tolerates 10X larger time steps

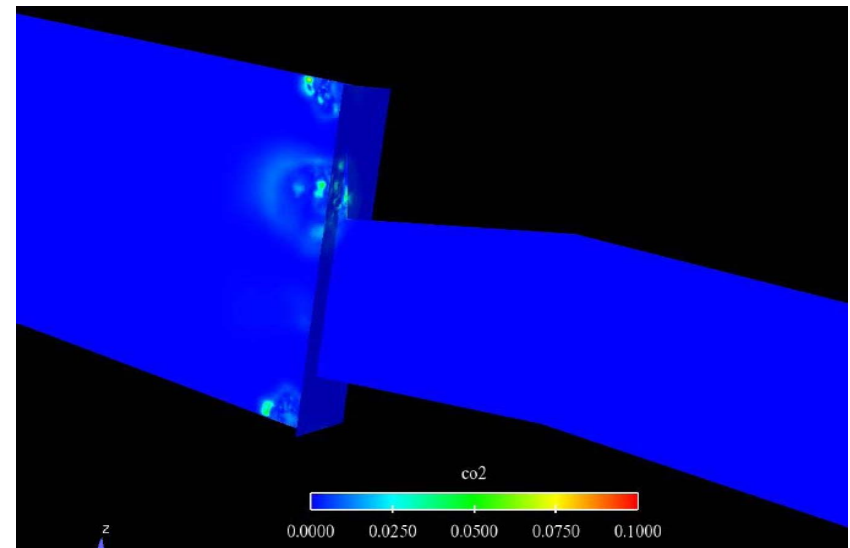
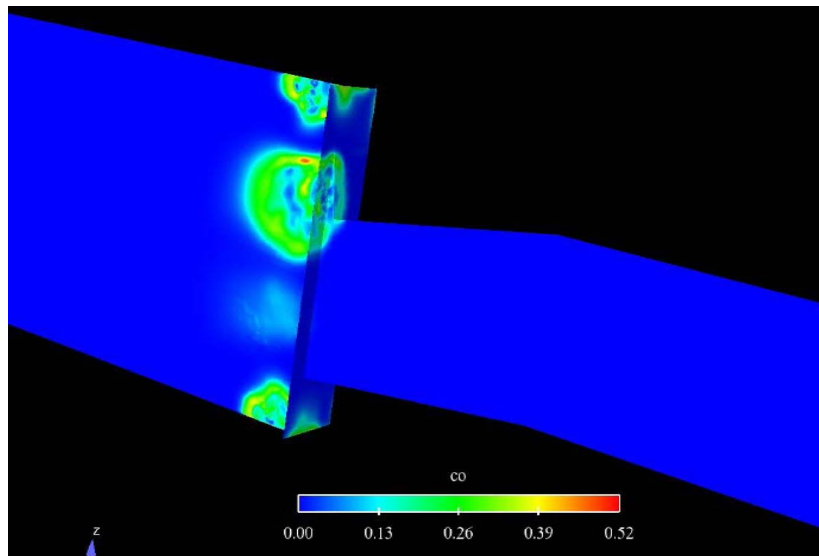


# Testimonial

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- Dr. Doug Lynch at Pratt & Whitney Rocketdyne:  
“This is the most stable hydrocarbon kinetics model I have ever used!”

The reduced model correctly captures the formation of CO before CO<sub>2</sub>.



Reaction Systems 23 species reduced mechanism for ethylene combustion

# Our Technology Produces Accurate Reduced Models from GRI Mech

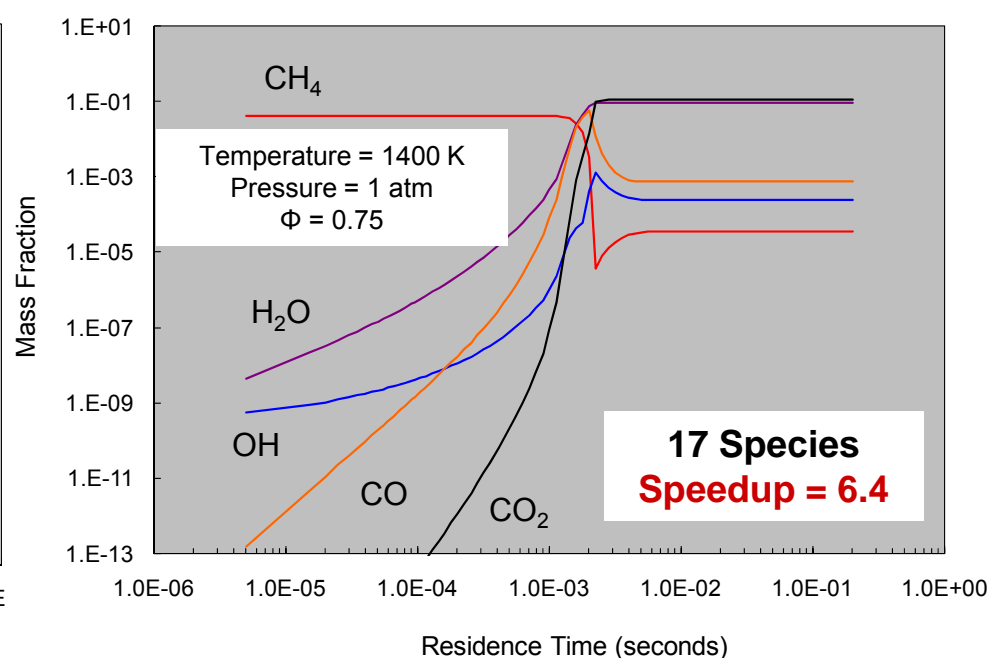
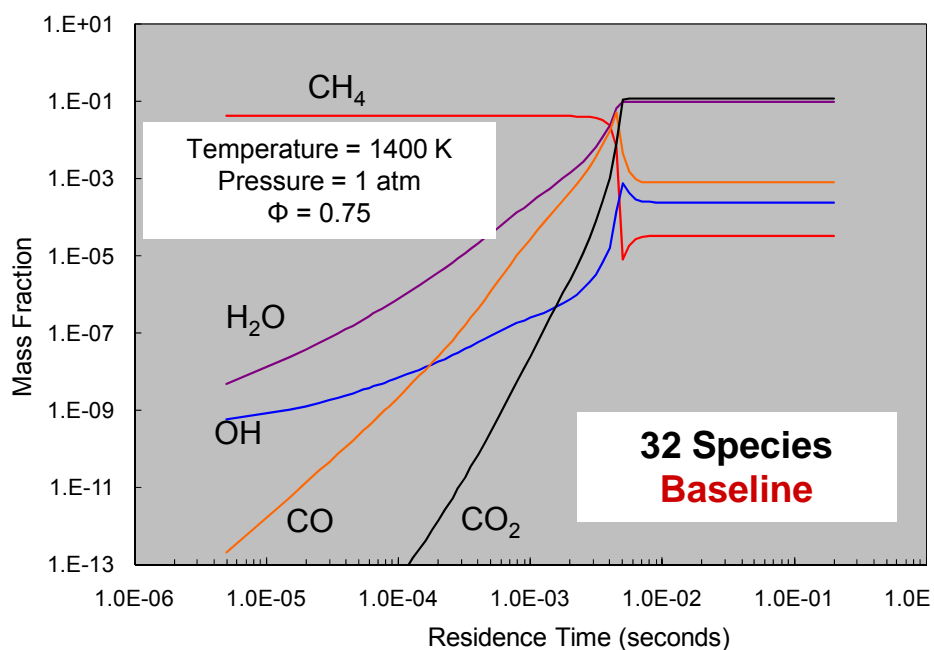
## Full GRI Mech 1.2

32 species; 117 reactions

## Reduced GRI Mechanism

17 species; 56 reactions

- Factor of 6.4 speedup!
- Very little loss in accuracy.
- Accurately predicts ignition time.

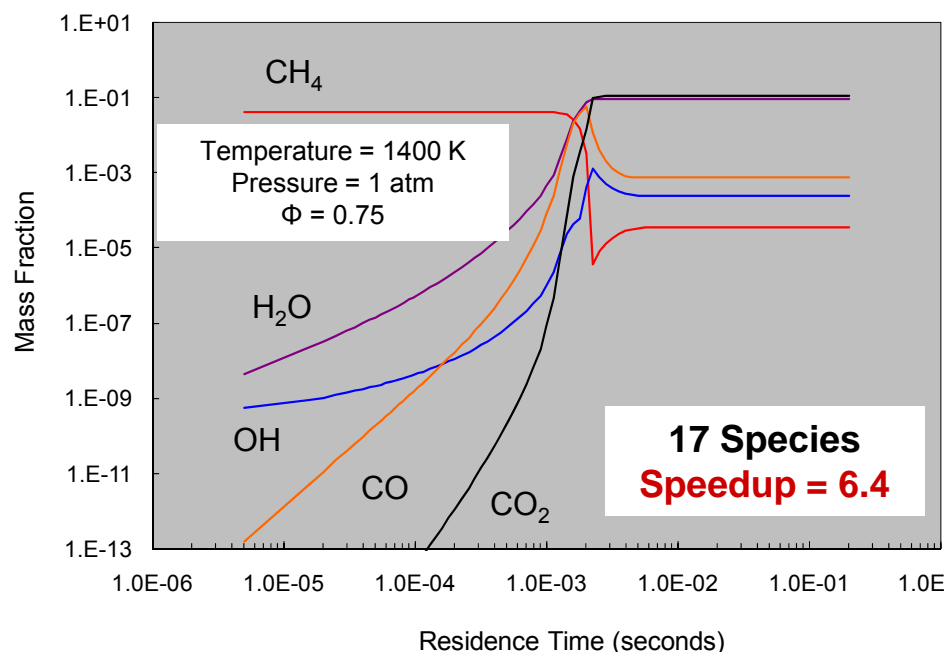


# Roadrunner Produces More Accurate Models than CARM

## Roadrunner Reduced GRI Mechanism

17 species; 56 reactions

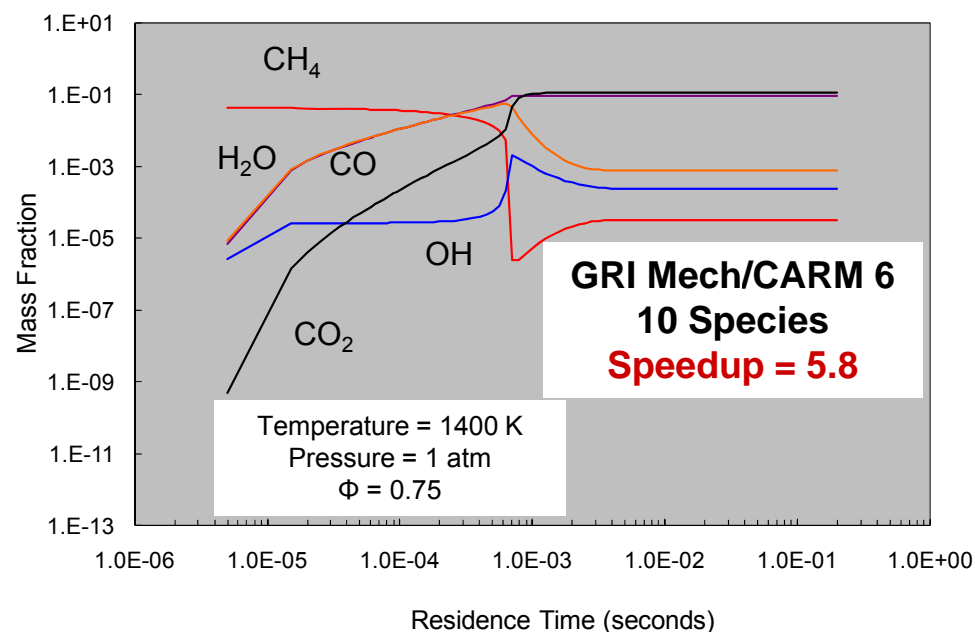
- Carries more species and runs faster than CARM.



## GRI Mech/CARM6\*

10 species; 6 reactions

- Less accurate and slower than our reduced model.
- Substantial error in ignition time.



\*CARM subroutines accessed at <http://firebrand.me.berkeley.edu/griREDU.html>

# *Why Our Mechanisms Are More Accurate*

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- We use the full mechanism to generate an extremely wide data base.
  - We developed codes that automate the process.
  - We include over 100,000 transient and steady state data points in our analysis.
- We then apply a unique approach to select the species that have the greatest impact on accuracy.
- Our data generation and species selection steps are automated; we can generate custom mechanisms that are tailored to fit the customers needs at minimal expense.

# *We Are Offering Custom Kinetic Mechanism Assembly & Reduction Services*

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- *Detailed Mechanism Assembly*
  - We compile species and elementary reactions from existing data bases.
  - We identify validation data and use only elementary reactions.
- *Reaction Systems Mechanism Reduction*
  - Our approach eliminates the least important species and reactions based on results obtained over a comprehensive data base.
  - It produces a hierarchy of reduced/skeletal mechanisms for consecutive implementation.
- *Reduced Mechanism Fitting*
  - We can adjust rate constants for improved fit to the data.
  - We can apply selected steady state assumptions to reduce stiffness and eliminate more species.
  - Reaction and species lumping to further reduce the number of species.



# *Contact*

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720-232-3597

See paper # AIAA 2009-5384