Roadrunner Kinetics
Custom Reduced Mechanisms for CFD

Reaction Systems, LLC • Golden, CO 80401 • www.reactionsystemsllc.com
Our Reduced Kinetic Models Have Superior Accuracy

Full Mechanism

Ethylene combustion
111 species; 781 reactions

Reduced Mechanism I
36 species; 216 reactions

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

Reaction Systems

\[ \text{Temperature} = 1200 \text{ K} \]
\[ \text{Pressure} = 1 \text{ atm} \]
\[ \Phi = 0.75 \]

- \( \text{C}_2\text{H}_4 \)
- \( \text{H}_2\text{O} \)
- \( \text{OH} \)

111 Species Baseline

36 Species Speed-up = 20
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

• 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 CO₂.

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/gredu.html
Why Our Mechanisms Are More Accurate

• 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

- **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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See paper # AIAA 2009-5384