“Kinetic mechanisms” discussion Summary

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Challenges

- Expense of theoretical and experimental determinations of rate coefficient
  - ~30 rate theoretical rate predictions / year; similar annual experimental yield
  - Not all theoretical predictions are of equal value; QC tools in the wrong hands can be dangerous

- Development and optimization of rate rules for reactions that can't be calculated or measured
  - Is number of rules finite?

Challenges

- Never will be enough data to validate a model across all conditions found in a turbulent flame
  - Need to identify regimes where uncertainty & sensitivity exists
  - Multiple groups perform complimentary experiments
  - (Re)evaluate old data
- At high temperatures
  - Pyroltic chemistry leaves fragments
  - Structure of fuel fragments (olefins) controls their reactivity
  - Design thoughtful experiment to probe these portions of the models; not always necessary to look at parent fuel
- Low temperatures: fuel specific chemistry important
- C_0 chemistry
  - Relatively small uncertainties (~25%) → high cost for small improvements
  - HO_2 chemistry a question, measurements needed

Challenges - What does industry care about?

- Real fuels
  - Blending effects – classes of components
  - Prediction of octane rating for fuel blends
  - Aromatics, olefins
  - N-alkanes (NTC energy release)
  - Alternative fuels farther off than public may think
- Mechanisms
  - Simplicity – number of reactions
  - Rate of heat release, transition from low- to high-T, temperature distribution, NOx, soot, noise (diesel), ignition delay
  - Resolve trends
  - Sensitivity of parameters on operation/performance
- Tools for: model development, surrogate formulation, rate prediction, etc.
  - Methods for dissemination and training
  - Industry is using: not predictive enough for computer design
    - No feedback
    - Little feedback even between kinetics and CFD communities
  - Translation of uncertainties in fundamental properties/predictions to uncertainties in applied outputs (engine performance)

How has the community changed?

- Today's perception: science will answer everything
- 1979: Irvin Glassman – "this soot problem keeps coming around"
  - Today – soot is still a problem
- First n-heptane mechanism ~1970
  - Still being worked on
  - First N-dodecane mechanism ~1990s
    - Similar fidelity to n-heptane
  - Still work need – NTC/low-T regions

Our work is directed by the problems facing industry

Roadmap/Collaborations

- Common community C_0 model
  - Optimized vs not
  - Dynamic vs fixed vs partially fixed
- Documentation
  - Data must be made available – necessary for simulation of exp
  - Models must be available, documented, and consistent (e.g., forward and reverse rates consistent with thermo)
  - Should further standardization of the requirements for reporting models and experiments exist?
- Cyber infrastructure for data/models/etc.
  - Models and data need to be on web
    - Improve the visibility of our work
    - Historical record of model changes
  - Prime?