Computational Modeling of Hypersonic Nonequilibrium Gas and Surface Interactions

Iain D. Boyd --- Grant No. (FA9550-11-1-0309) --- University of Michigan

Analysis of High-Temperature Chemical Kinetics Using Rates Computed at Molecular Level

STATUS QUO

State-of-the-art thermo-chemistry models for hypersonic flow analysis

- Usually consider relaxation of the vibrational energy mode, omitting effects of rotational energy
- Assume simplified effect of vibration on rate of dissociation, and vice versa
- Development of more sophisticated approach requires evaluation of rates for large number of coupled processes

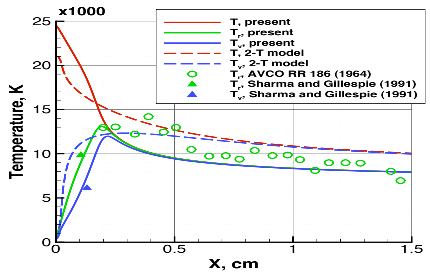
NEW INSIGHTS

NASA Database Used to Study Nitrogen Interactions (N_2-N)

- Interactions analyzed at molecular level using computational chemistry
- Allows extension of high-temperature thermochemical models to include all relevant processes
- Evaluation using several sets of existing experimental data

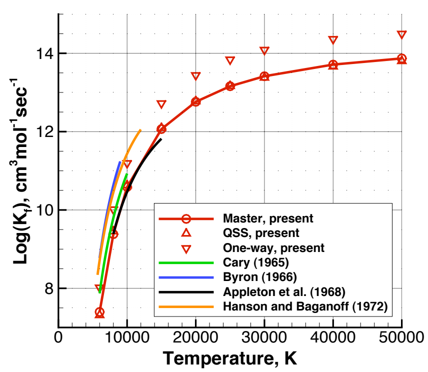
Representative hypersonic vehicle

MAIN ACHIEVEMENTS:



Detailed master equation analysis of shock tube experiments allows evaluation of new models

• NASA database of state-resolved rates extended to high temperature • State-to-state rates of rotational, vibrational, and chemical transitions obtained and employed in master equation analyses • Rates used to perform detailed transient analyses to derive macroscopic information such as relaxation parameters • Rates also applied to analyze 1d shock tube flows for comparison with measurements

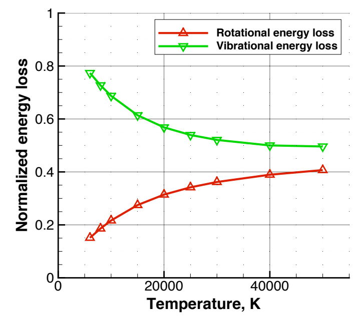


Dissociation rate of N_2-N: comparisons of computed and measured data

QUANTITATIVE IMPACT

Current Impact

• 9,390 differential equations solved simultaneously • Allows detailed study of all thermochemical processes of N_2-N • Relatively simple flow analyses to investigate detailed nonequilibrium relaxation phenomena



Average energy removed from different energy modes during nitrogen dissociation

Planned Impact

• Process will be repeated for additional thermochemical processes in air • Larger number of interactions must be considered • Detailed comparisons with high-temperature experiments

END-OF-PHASE GOAL

Research Goals

• Data base of thermochemistry rates for all processes in air • Analysis of relaxation phenomena to identify reduced order models for CFD • Implementation of models in CFD code and evaluation through application to hypersonic flows

Highlight Slide Template

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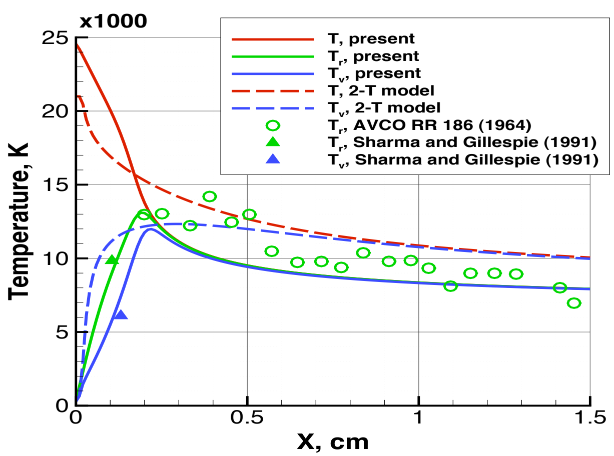
Headline: Detailed analysis of high-temperature chemical kinetics made possible using optimization approach



- Heating of hypersonic vehicles is influenced by high temperature chemistry
- Current chemistry models ignore a large number of important processes due to a lack of rate data
- NASA database used in detailed analysis of nitrogen (N_2-N) interactions
- Models evaluated using existing experimental data[1]

Iain D. Boyd

James E. Knott Chair of Engineering

- Fellow of Am. Inst. Aero. Astro. (AIAA)
- 1998 AIAA Lawrence Sperry Award
- 2011 AIAA Thermophysics Best Paper Award
- AFSAB member

[1]Kim & Boyd, AIAA Paper 2012-3305, June 2012

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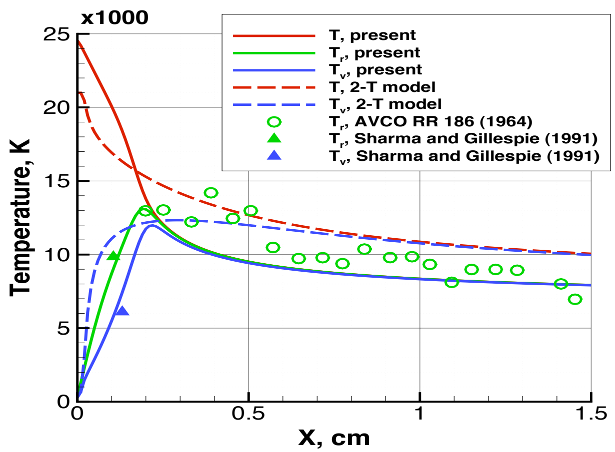

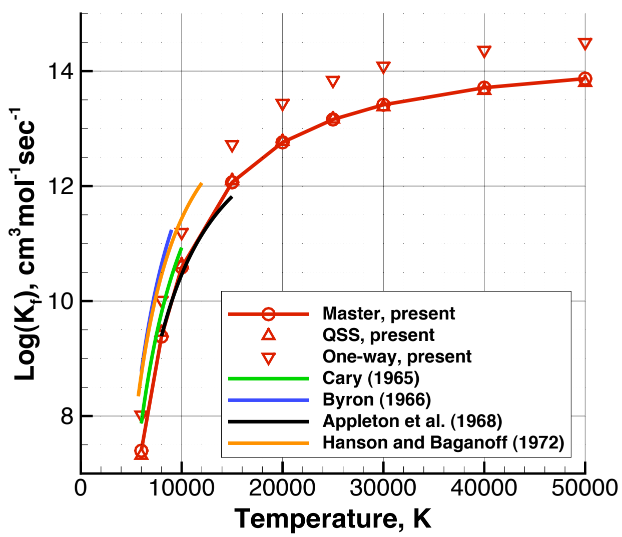

Use of detailed NASA database for nitrogen interactions enables simulation of high-temperature thermochemistry for all relevant processes with evaluation based on experimental measurements[1]

Computational chemistry used to generate cross sections that are integrated to rates

Rates using in 9,391 simultaneous equations to analyze all thermochemical processes

Computation of shock tube flows provides new insight into nonequilbrium phenomena and good agreement with measured data

[1]Kim & Boyd, AIAA Paper 2012-3305, June 2012

Heilmeier's Catechism

Your Highlight Should Answer *the Red* Questions – green (2nd priority) and black (3rd priority) questions are nice, but optional

by George H. Heilmeier, President and CEO of Bellcore

- What are you trying to do? Articulate your objectives using absolutely no jargon.
- How is it done today, and what are the limits of current practice?
- What's new in your approach and why do you think it will be successful?
- Who cares? If you're successful, what difference will it make?
- What are the risks and the payoffs?
- How much will it cost? How long will it take?
- What are the midterm and final "exams" to check for success?

Additionally…

- Does this work address the objectives of the portfolio to which it is being submitted?
- Are there opportunities to collaborate with other efforts – both internally and externally?