Agenda: Fundamental Processes in High-Temperature Hypersonic Flows

8:30	--	8:40	John Schmisseur: Introduction
8:40	--	9:00	Graham Candler: Overview
9:00	--	10:30	Truhlar / Candler Group
10:30	--	11:00	Break
11:00	--	11:30	Adri van Duin
11:30	--	12:00	Tom Schwartzentruber
12:00	--	1:30	Lunch
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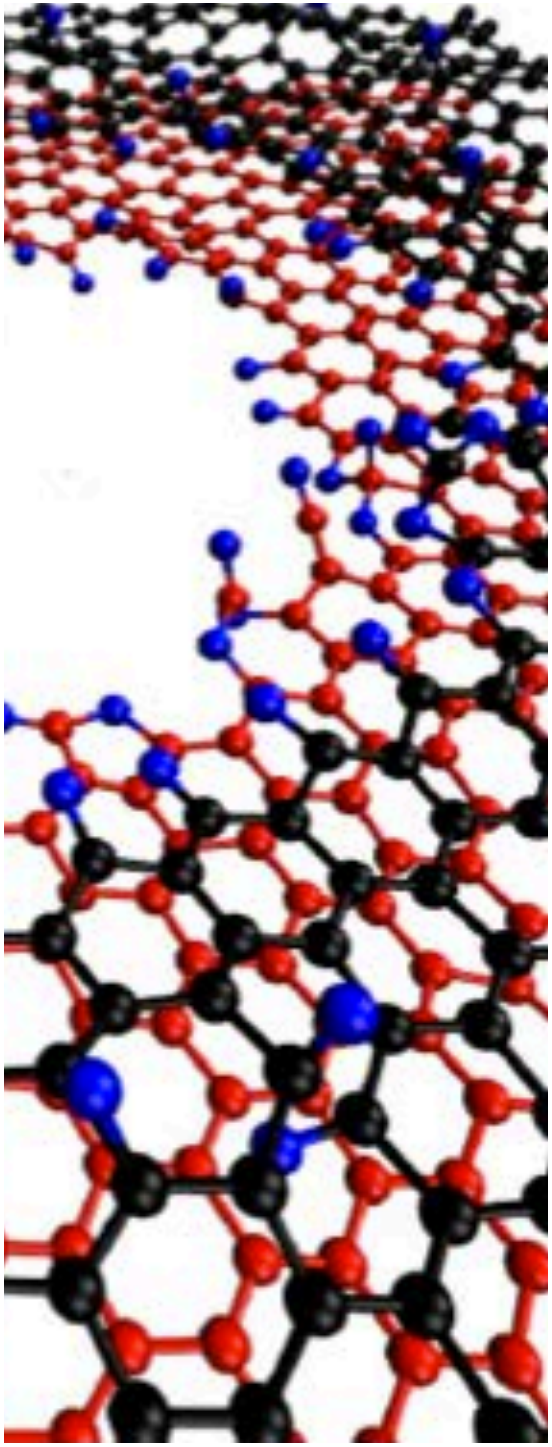
4:00	--	4:30	Graham Candler



Fundamental Processes in High-Temperature Hypersonic Flows

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Aerospace Engineering & Mechanics
University of Minnesota

Support from AFOSR

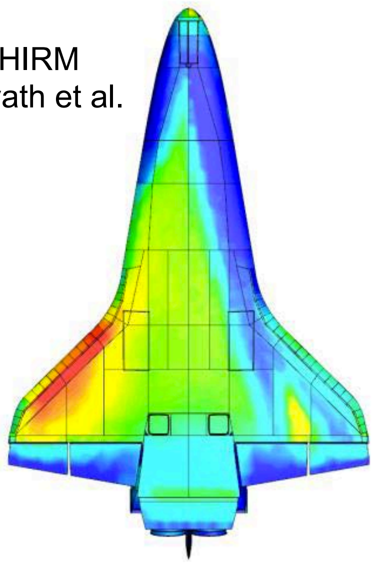
Program Managers:
Michael Berman, Ali Sayir, and John Schmisseur

MURI Review

July 15, 2013

Problem Statement and Goals

HYTHIRM
Horvath et al.



Typical Flow Conditions:

Gas T ≈ 10,000 K, solid T ≈ 4,000 K

Chemical reactions, ionization, gas-surface interactions

Non-equilibrium processes; rate driven

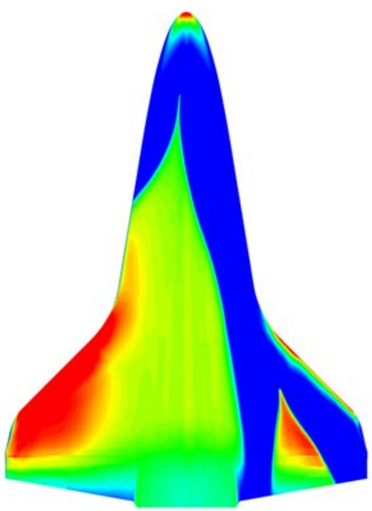
All models must be valid and consistent

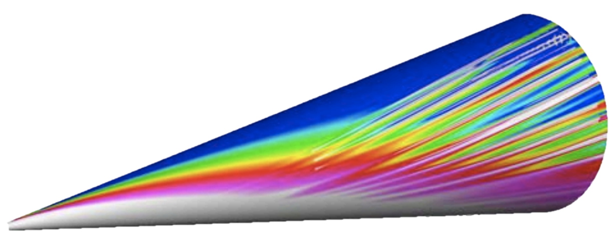
Goals:

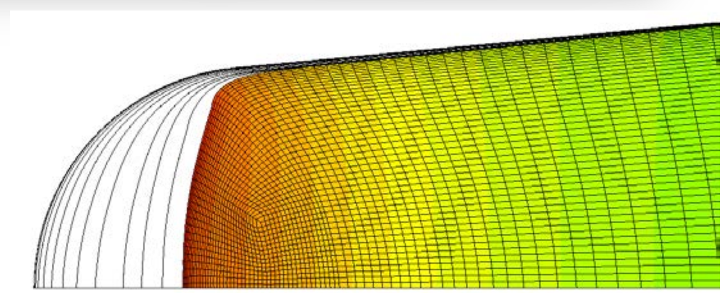
Understand the fundamental physics of these processes

Develop accurate models; control; design new materials

> We're really good at solving the equations;
> The biggest uncertainty is in the rates/mechanisms…







Available Gas-Phase Kinetics Data

- Rates from experiments in the 1960s and 70s:

Inferred rates depend on the model used to interpret the data

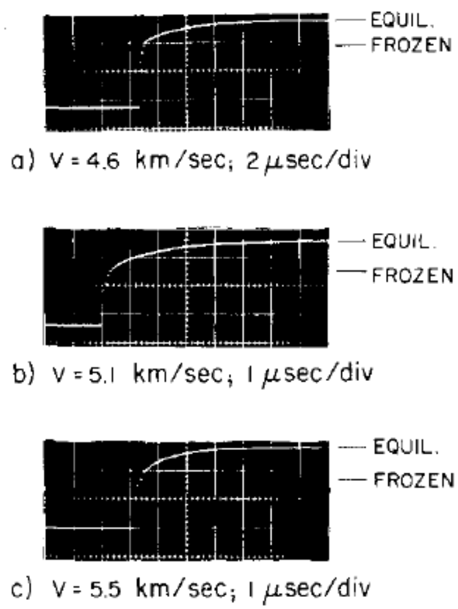
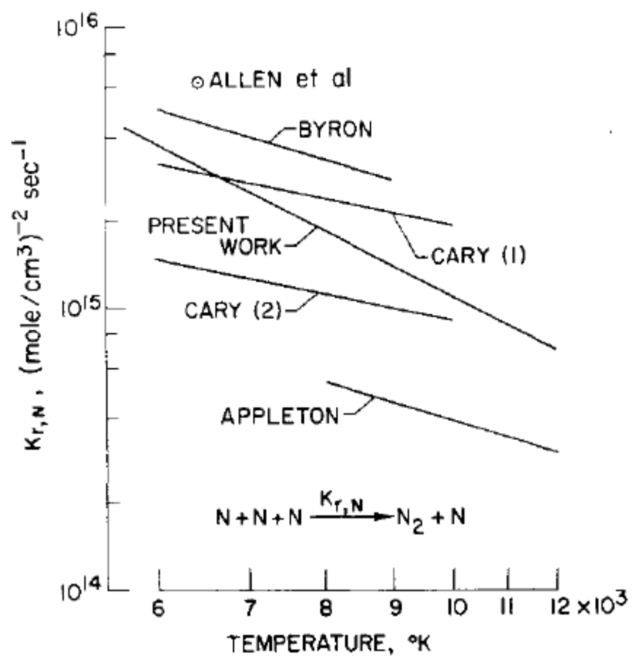
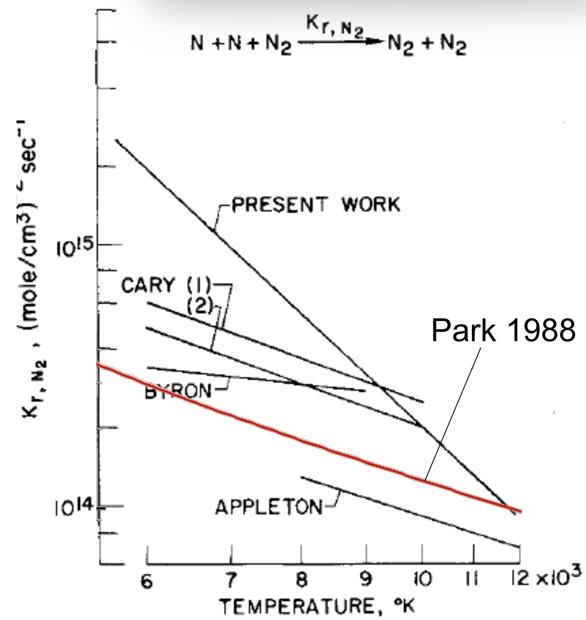


Fig. 1 **Pressure-gage data for N_2 at 2.1 torr.**



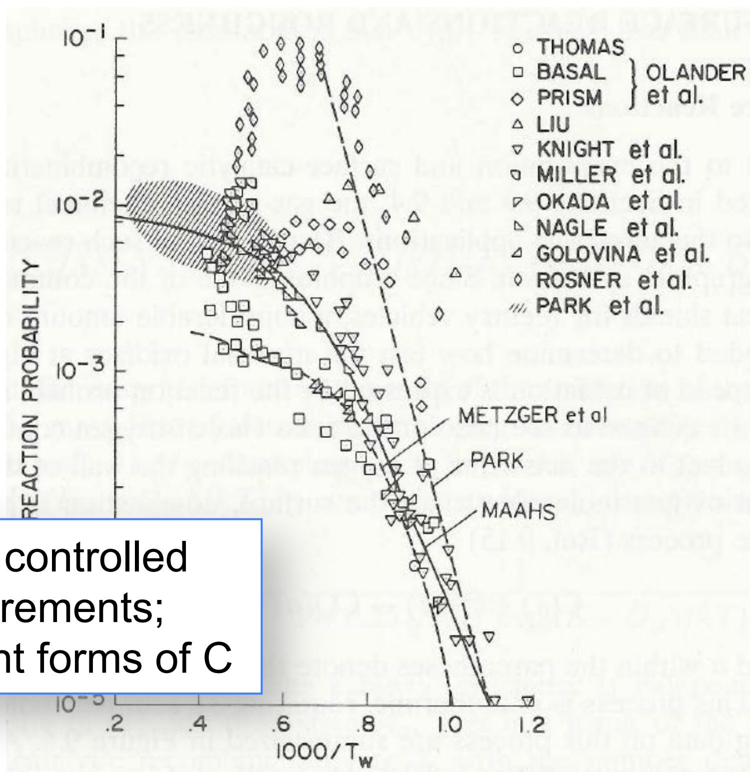


Hanson and Baganoff (1972): Dissociation rates inferred from end-wall pressure measurements in a shock tube.

Park (1988) re-interpreted the data using his two-temperature model.

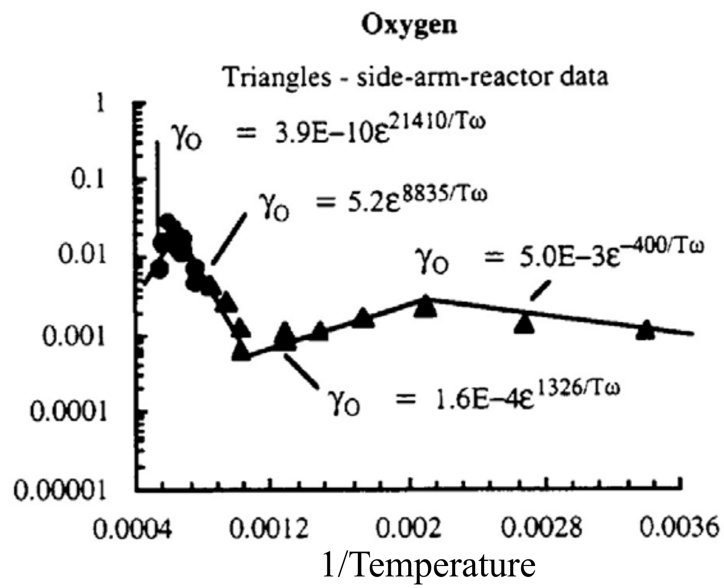
Gas Surface Interaction Modeling

- Existing models for oxidation and catalysis exhibit large variations
- Mechanisms cannot be inferred from experiments alone
- Bridge from detailed chemistry to macroscopic rates



Poorly controlled measurements; different forms of C

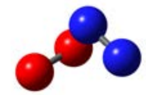
Rate data for $C(s) + O_2 \rightarrow CO_2$ on carbon and current models



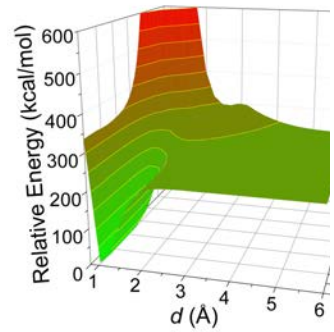
Oxygen recombination efficiencies on RCG silica-based tiles (Stewart 1997)

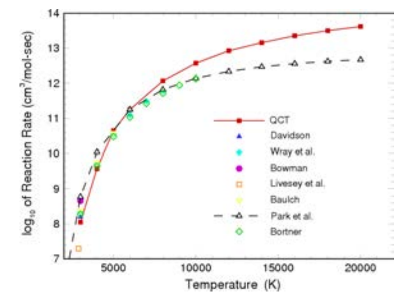
Data from poorly characterized arc-jets

Approach / Goals

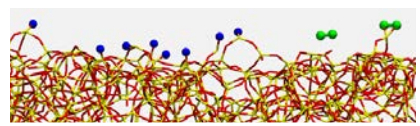

CASPT2

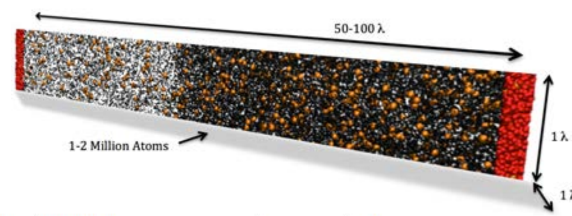
- Apply scientific methods to a field long dominated by empiricism





- Combine:
  - Computational chemistry
  - Numerical simulations
  - Experiments
  - Full range of scales

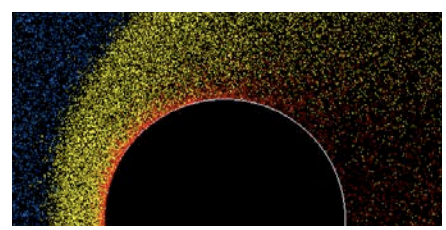


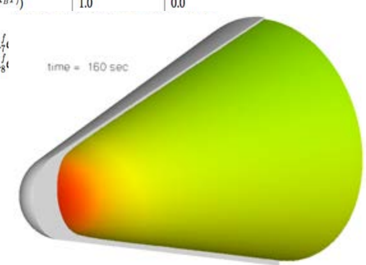


- Improve the fundamental understanding of high-temperature processes

Rate	Rate Equation	Functional Form	A	E_a (eV)
r_1^f	$k_1^f[O][E_s]$	$(\bar{c}_O/4) \times (2\pi r_s^2) \times (A_1^f e^{-E_1^f/(K_B T)})$	1.0	0.0
r_1^r	$k_1^r[O_s]$	$A_1^r e^{-E_1^r/(K_B T)}$	10^{-15} (s^{-1})	4.25
r_2^f	$k_2^f[O][O_s]$	$(\bar{c}_O/4) \times (2\pi r_s^2) \times (A_2^f e^{-E_2^f/(K_B T)})$	0.169	0.401
r_2^r	$k_2^r[O_2][E_s]$	$(\bar{c}_{O_2}/4) \times (2\pi r_s^2) \times (A_2^r e^{-E_2^r/(K_B T)})$	0.663	1.27
r_3^f	$k_3^f[O][O_s]$	$(\bar{c}_O/4) \times (2\pi r_s^2) \times (A_3^f e^{-E_3^f/(K_B T)})$	1.13	0.253
r_3^r	$k_3^r[O_{2s}]$	$A_3^r e^{-E_3^r/(K_B T)}$	10^{-15} (s^{-1})	4.14
r_4^f	$k_4^f[O][O_{2s}]$	$(\bar{c}_O/4) \times (2\pi r_s^2) \times (A_4^f e^{-E_4^f/(K_B T)})$	0.172	0.303
r_4^r	$k_4^r[O_2][O_s]$	$(\bar{c}_{O_2}/4) \times (2\pi r_s^2) \times (A_4^r e^{-E_4^f/(K_B T)})$	0.716	1.18
r_5^f	$k_5^f[O_{2s}]$	$A_5^f e^{-E_5^f/(K_B T)}$	1.20×10^{14} (s^{-1})	2.71
r_5^r	$k_5^r[O_2][E_s]$	$(\bar{c}_{O_2}/4) \times (2\pi r_s^2) \times (A_5^r e^{-E_5^r/(K_B T)})$	1.0	0.0
r_6^f	$k_6^f[O][E_f]$	$(\bar{c}_O/4) \times (2\pi r_s^2) \times (A_6^f e^{-E_6^f/(K_B T)})$	1.0	0.0
r_6^r	$k_6^r[E_f]$	$(A_6^r e^{-E_6^f/(K_B T)})$		
r_7^f	$k_7^f[O][O_f][E_c]$	$(2\pi r_s \Lambda_D) \times (\bar{c}_O/4) \times P_{rc} \times (A_7^f$		
r_8^f	$k_8^f[O][O_f][O_c]$	$(2\pi r_s \Lambda_D) \times (\bar{c}_O/4) \times P_{rc} \times (A_8^f$		

- Develop a rigorous approach for modeling gas-surface interactions





MURI Team

PI - Graham Candler: Non-equilibrium CFD modeling

Tom Schwartzentruber: MD and DSMC modeling

Don Truhlar: Quantum chemistry and reaction dynamics

Dan Kelley: Nonequilibrium chemistry theory and modeling

Adri van Duin: Classical MD; reactive force fields

Debbie Levin: thermal radiation analysis; DSMC

Tim Minton: Molecular beam experiments

Erica Corral: Materials fabrication and experiments, UHTCs

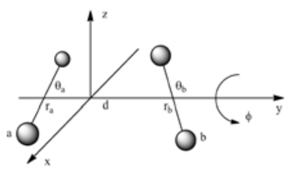
Paul DesJardin, Matthew Ringuette, and **Matt MacLean**:

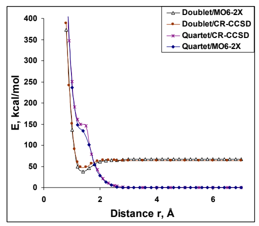
High-enthalpy full-scale experiments

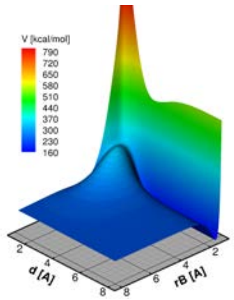
MURI Team Interactions

Gas-Phase Kinetics Modeling:

Truhlar / Candler / Levin

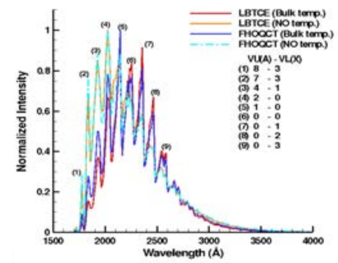


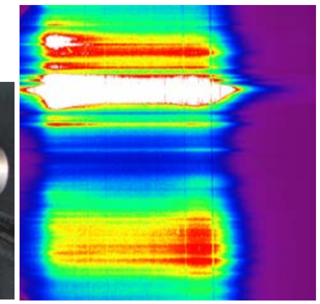




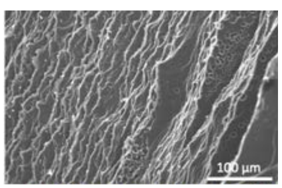
Radiative Emission Measurements / Theory:

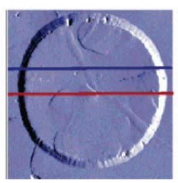
UB / Levin / Candler

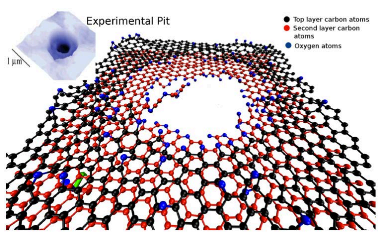




Graphite Experiments / Gas-Surface Modeling: Corral / Minton / van Duin / Schwartzentruber / Candler

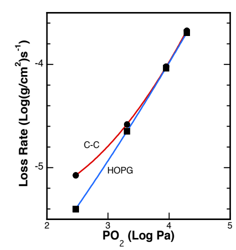


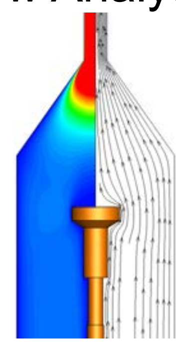




Nonequilibrium TGA Flow Analysis:

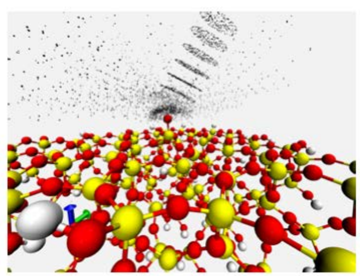
Corral / Candler





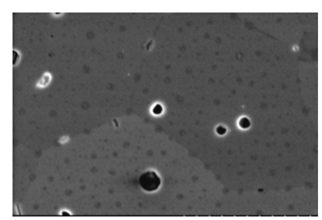
Silica-Oxygen Gas-Surface Interaction Modeling:

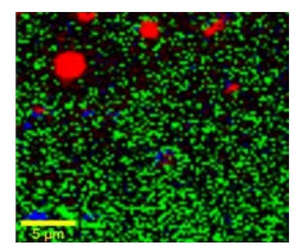
Truhlar / van Duin / Schwartzentruber



UHTC Experiments:

Corral / Minton





Scientific Accomplishments / Breakthroughs

- N_4, O_4, N_2O_2 potential energy surfaces at relevant conditions
- Novel potential energy surface fitting approaches
- Parallelization and upgrades of ANT trajectory code
- Shock-layer radiation emission measurements at flight conditions
- ReaxFF modeling of graphite gas-surface interaction
- CFD analysis of Dynamic Nonequilibrium TGA
- Molecular beam measurements of UHTCs and graphite at high T
- Sensitivity of shock layer flows to detailed rate processes
- Potential universal carbon oxidation mechanism

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