Computational Modeling of Hypersonic Nonequilibrium Gas and Surface Interactions

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Hypersonic Vehicle Analysis

Gas Phase
- strong shocks, thermochemical nonequilibrium, boundary layer, etc.
- CFD, relaxation times, Arrhenius rate coefficients with two-temperature model

Surface Processes
- accommodation, ablation (oxidation, sublimation), catalysis, melting, etc.
- coefficients, surface chemistry mechanism and rates

Material Response
- heat conduction, radiative emission, internal chemical reactions (pyrolysis), gas flow through porous media, etc.
- thermal response model, physical properties of complex materials (conductivity, emissivity…)

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Material Response
Project Goals

• Nonequilibrium gas-phase processes:
  – use computational chemistry and Master Equation analysis to perform detailed studies of:
    • thermal relaxation processes (T-R-V)
    • chemical processes (dissociation, exchange)
  – develop reduced order models for use in CFD

• Nonequilibrium gas-surface processes:
  – use coupled CFD-surface chemistry-material response tools to study gas-surface interactions (e.g., catalysis, ablation)
  – assess models using experimental data (flow and surface) generated in high-enthalpy facility (Fletcher, Univ. Vermont)
Gas Phase Studies: Technical Approach

• State-to-state transition cross sections and rate coefficients:
  – compute data for all ro–vibrational states, e.g. using QCT
  – reduce the number of state-to-state transition rates evaluated using a response surface design technique (Kriging)

• Master Equation (ME) analysis of thermochemical relaxation:
  – constructed using complete sets of state-resolved transition rates for bound-bound and bound-free processes
  – compare results with existing measurements
  – use results to develop reduced-order thermochemistry models that can be implemented in CFD
Results:
Bound-Bound H₂ Transitions

State-to-state cross sections obtained using response surface design method.
Results:
Bound-Bound H\(_2\) Transitions

State-to-state cross sections obtained using response surface design method calibrated using a small number of QCT evaluations (1,800 instead of 60,000!)

(a)
(b)
Results: H₂ Thermal Relaxation

- Global relaxation parameters of the rotational and vibrational modes for H₂+H₂
- Rotational and vibrational relaxation times become similar at high temperature
Analysis of N₂-N: Heat Bath Studies

- State-to-state transition cross sections and rate coefficients:
  - use database of cross sections computed by Jaffe et al, NASA ARC
  - ME analysis involves solution of 9,390 equations
  - technical details: Kim & Boyd, AIAA-2012-2991, June 2012

Thermal Relaxation Parameters

Chemical Reaction Rates

Energy Removal Due to Chemistry
Analysis of N$_2$-N: Shock Tube Studies

- One-dimensional flow equations combined with Master Equation:
  - N$_2$-N$_2$ included macroscopically using standard models
  - applied to experiment of AVCO / Sharma
  - technical details: Kim & Boyd, AIAA-2012-2991, June 2012
Gas-Surface Interactions: Assessment of Computations

- Collaboration with Prof. Doug Fletcher (UVM):
  - 30 kW Inductively Coupled Plasma (ICP) Torch Facility
- Samples exposed to high enthalpy gas flows
- Flow quantities measured using two-photon LIF:
  - N-atom number density
  - Translational temperature
- Surface temperature and sample ablation also quantified

Graphite sample in nitrogen flow
(section in box is the portion simulated)
Source: Prof. D.G. Fletcher
Gas-Surface Interactions: Conditions Investigated

Free Stream:

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<td>0.001</td>
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<td>12</td>
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</tr>
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</table>

Progress: subsonic inlet/outlet BCs added to LeMANS sensitivity to various thermochemistry models

Mach number

Translational temperature
Gas-Surface Interactions: Comparisons with Experiment

Comparisons along the stagnation streamline

Translational temperature

Relative N-atom density
Future Plans

• Nonequilibrium gas-phase processes:
  – develop T-R-V relaxation models for CFD from ME results
  – high fidelity CFD chemical reaction models including rotational mode will also be developed from ME analysis
  – continue analysis for other important air interactions
  – evaluation using existing experimental data sets

• Nonequilibrium gas-surface processes:
  – compare surface chemistry models (catalytic recombination, finite rate chemistry module of MacLean & Marschall)
  – model surface recession (material response code: MOPAR)
  – study sensitivity to gas-thermochemistry rates and models
  – assess modeling using Univ. Vermont experimental measurements of flow field properties and sample mass loss
Technical Challenges

• Nonequilibrium gas-phase processes:
  – large number of different air species interactions (N₂-M, O₂-M, NO-M, etc.)
  – fidelity required from computational chemistry?
  – Master Equation analysis becoming expensive
  – lack of modern, validation quality, experimental data

• Nonequilibrium gas-surface processes:
  – isolating contributions of competing mechanisms to effects observed (e.g. flow processes, catalysis, ablation)
  – uncertainties in facility operation (e.g. ICP exit conditions)
Technical Approach: Computational Tools

• **LeMANS**
  (Scalabrin and Boyd: AIAA-2006-3773)
  - Navier-Stokes CFD code
  - finite volume FVS
  - implicit time integration (point/line)
  - 2D/3D unstructured mesh
  - parallel, domain decomposition
  - finite rate thermo-chemical nonequilibrium effects
  - validated for hypersonic flow using experiments, codes

• **MOPAR**
  (Martin and Boyd: AIAA-2009-3597)
  - material response code
  - control volume finite element (CVFEM)
  - quasi-1D
  - pyrolyzing/non-pyrolyzing ablators
  - momentum conservation through Darcy’s Law (or Forcheimer’s Law)
  - moving boundaries
  - has been coupled to LeMANS
Results: Surface Properties

Total Heat flux = (Translational + Vibrational) convective heat flux + Diffusive heat flux

![Graphs showing Total heat flux and Diffusive heat flux vs Distance from stagnation point]