Nonequilibrium Gas Dynamics: Understanding of High-Speed Flows at Strong Energy Mode Disequilibrium

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Seminar at the Department of Aeronautical Engineering

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NETL Group

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Scope of Research

• **Generation and sustaining of stable high-pressure weakly ionized plasmas**

• **High-speed flow control by nonequilibrium plasmas / MHD**

• **Ignition, combustion, and flameholding by nonequilibrium plasmas**

• **Molecular gas lasers**

• **Kinetics of gases, plasmas, and liquids at extreme thermodynamic disequilibrium**

• **Molecular energy transfer processes: excitation and relaxation of vibrational and electronic levels, chemical reactions among excited species, plasma radiation**

• **Electron and ion kinetics: ionization, recombination, electron attachment and detachment, charge transfer, inelastic electron-molecule collisions**

• **Flow visualization and optical diagnostics**
“Air Plasma Ramparts Using Metastable Molecules” (AFOSR MURI '97-'02)

“Anomalous Shock Wave Propagation and Dispersion in Weakly Ionized Plasmas” (AFOSR '99-'01, NASA '99-'00)

“Effect of Vibrational Nonequilibrium on Electron Kinetics in High Pressure Molecular Plasmas” (NSF/DOE, '00-'06)

(AFRL/DAGSI, '01-'03) “Non-Thermal Ignition Phenomena for Aerospace Applications”

“Generation and Characterization of Stable, Weakly Ionized Air Plasmas in Hypersonic Flows” (AFRL/DAGSI, '01-'03)

“Energy Transfer Rates and Mechanisms for Hypervelocity Vehicle Radiation” (AFOSR, '01-'07)

“Effect of MHD Forces on Stability and Separation of Nonequilibrium Ionized Supersonic Flow” (AFOSR, '02-'04)

“Plasma Flow Control Technology for Hypersonic Boundary Layer Transition Control” (AFRL, '02-'05)

“Electric Discharge Oxygen-Iodine Laser” (AFRL, '04-'06)
“Plasma Assisted Ignition Module for Aerospace Propulsion Systems” (AFOSR, '04-'06)

“Nonequilibrium Supersonic Magnetogasdynamic Wind Tunnel” (AFOSR, '05-'07)

“Instrumentation for Generation and Optical Diagnostics of Repetitively Pulsed Fast Ionization Wave Plasmas in Supersonic Flows” (AFOSR DURIP, '05-'06)

“Active Control of Jet Noise Using Plasma Actuators” (NASA '02, '05-'06, with GDTL)

“Electric Discharge Oxygen-Iodine Laser Operating at High Pressure” (JTO, '06-'08)

“Kinetic Studies of Plasma Assisted Combustion By Non-Equilibrium Discharges” (AFOSR, '07-'09)

“Nonequilibrium Ignition and Flameholding in High-Speed Reacting Flows” (NASA, '07-'09)

“Supersonic Jet Noise Suppression Using Plasma Actuators” (NASA '07-'09, with GDTL)

“Nonequilibrium Gas Dynamics” (AFOSR '08-'10)
NETL Research in Broader Context:
National Hypersonic Basic Research Plan (AFOSR, NASA, SNL)

Thrust Areas

• Boundary Layer Physics

• Nonequilibrium Flows*

• Shock-Dominated Flows

• Environment-Material Interactions

• High-Temperature Materials

• Supersonic Combustion*

* studied in NETL
Critical System Impact of Nonequilibrium Hypersonic Flows

• TPS Design: Current uncertainties for reacting air (and other gases) at re-entry and cruise create estimated factor of two errors in predicting heat load and designing leading edges, TPS

• Aerodynamic Control: High-altitude aerodynamics including pitching moments and reaction control systems/surfaces not predictable. Wake heating and large angle-of-attack flows not predictable
Nonequilibrium Hypersonic Flows: Key Technical Issues

Boundary Layer
Transition
Very High AoA
Aerodynamics
Ablation Small-Scale
Geometric Effects
Plasma/Comm
Issues
Very High AoA
Aerodynamics
Leading Edges
and RCS
Wake Flow & Separation
Dynamics
Global Strike /
Responsive Space
Aerothermodynamic
plasma generation
Stagnation
Heating
Ablation
Small-Scale
Geometric Effects
Planetary Entry
Space Situational Awareness:
track/ID unknown missiles / satellites
using their EM signatures

Plasma blackout:
plasma generated by hypersonic flow
blocks telemetry – big issue for both
development and operation
How Good is the Current State of the Art (SOA)?

Temperature behind a 12 km/sec shock predicted by SOA model is not even close to experiment (in pure nitrogen!)

Matsuda et al, JTHT, 2004

Static temperature and NO fraction predicted by SOA model in a M=15 expansion “air” flow are off.

Experiment: LENS, M=15, run time ~1 msec

Candler et al, AIAA Paper, 2007

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow velocity, m/s</td>
<td>4517</td>
</tr>
<tr>
<td>Temperature, K</td>
<td>250-300</td>
</tr>
<tr>
<td>NO fraction, %</td>
<td>1.5</td>
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</table>

We have a problem (might be both with experiment and modeling)

Basic research vision for the next 30 years must include development and validation of design tools that simulate hypersonic vehicle aerothermodynamics and propulsion
Key Challenges

• Due to shock waves, boundary layers, or rarefaction, concept of single temperature breaks down, fluid dynamic equations break down, chemistry is not well understood.

• Understanding / predicting these flows requires insight into molecular / surface / radiation / plasma interactions.

• Four interacting research areas:
  - Basic chemical physics
  - Ground test, flight data: Facilities, advanced diagnostics
  - Simplified “good enough” models: gases, gas-surface, plasma
  - Aerothermo simulations: speed, validity

Need to predict nonequilibrium hypersonic flows based on sound physics, not extrapolations of measurements or empirical correlations.
Strategic (Long Term) Goals

Foster development of both technical and human resources for the exploration, characterization and control of flows at high Mach numbers with significant thermochemical nonequilibrium.

• **Development of validated physics-based tools** for prediction of heating, aerodynamics, etc of hypersonic system

• **Transfer** of proven, physics-based models and simulation methods and complementary technical expertise to industry and applied research

• Development and maintenance of **essential human resources** to capitalize on and continue progress in this area.
Objectives Defined by Nonequilibrium Thrust Panel at NASA / Air Force Workshop, June 2007

Near term (<5 years):

- Measure key air reaction rates and mechanisms at higher temperatures
- Develop improved catalytic wall-boundary condition for hypersonic flow with typical surface
- Plan, design, fund facilities for well-characterized reacting hypersonic flow data
- Obtain ground and/or flight data with spectral, species, or spatially-resolved reacting hypersonic flow. Utilize/coordinate with NATO RTO results

Mid-term (5-10 years):

- Measure / accurately calculate all important atmospheric (earth/other) gas reactions at ultra-high temperatures
- Validate advanced ultra-high temperature models for excited states, relaxation, surface collisions, catalysis, ablation
- Complete integrated radiation transport models; accurate ultra-high temperature gas transport properties
- Well-characterized reacting hypersonic flow data using advanced diagnostics
- Fast CFD and kinetic simulation tools with integrated physics models
NETL Contribution: Outline

I. Ability to generate and sustain steady-state supersonic flows with strong energy mode disequilibrium and targeted energy loading

II. In-depth flow characterization using advanced optical diagnostics

III. Physics-based, validated molecular energy transfer and nonequilibrium chemical reaction models

IV. New research program: characterization of nonequilibrium supersonic flows, developing instrumentation for use at a national hypersonic facility (LENS)

V. Future research thrusts
A Bit of History:
Shock Weakening by Weakly Ionized Plasmas

Ballistic range / glow discharge experiments

(Russia, 1980’s; U.S., 1990’s)

- shock stand-off distance increases
- wave drag reduction up to 50%

Suggested Interpretations

- vibrational relaxation
- ion-acoustic wave
- nonuniform heating

Bow shock around a sphere.
Air, P=9.5 torr, u=1600 m/s
(AEDC, 1999)
Case 1: Steady State Plasma Shock Experiment

Aerodynamically Stabilized DC Glow Discharge

Transverse RF discharge electrodes

Wedge

Anode
Cathode

Nozzle
Test Section
Diffuser
M=2 plasma flows with and without RF ionization

\[ P_0 = 250 \text{ torr}, \]
\[ \text{N}_2/\text{He}=50/50 \text{ mixture}, \]
\[ P_{\text{test}} = 48 \text{ torr} \]

RF discharge off
\[ n_e \sim 10^9 \text{ cm}^{-3} \]

RF discharge on
\[ n_e = (1-3) \cdot 10^{11} \text{ cm}^{-3} \]

Stable, uniform, and diffuse plasmas in both cases
Shock weakening by the RF plasma:
\[ \Delta \alpha = 15^0, \Delta M = -0.2 \]

Slow shock weakening and recovery: thermal effect
Flow temperature measurements
(CO FT infrared emission spectroscopy – with 4% CO added)

Almost no core flow heating by the discharge
Noticeable boundary layer heating
Temperature measurements summary

Rotational temperature, K

- Low J' fit (J'=1-12)
- High J' fit (J'=12-19)
- Fit to all data (J'=1-19)

$\Delta T=15 \text{ K (low J'}$ fit

$\Delta T=50 \text{ K (high J'}$ fit

$\Delta T=35 \text{ K (all available data fit)}$

Temperature rise consistent with shock angle change ($\Delta M=-0.2$ for both)

Thermal effect
Case 2: Supersonic Flow Control by Low-Temperature MHD

- Pulsed electric field perpendicular to the flow, parallel to magnetic field
- DC sustainer field perpendicular both to flow and pulsed electric field
- Optical access along vertical and horizontal line-of-sight
- Four combinations of current and magnetic field directions: Accelerating or decelerating Lorentz force, \( j \times B \)
Low-temperature MHD test sections (M=3, M=4)

- Contoured nozzle
- 12 cm long, 4 cm x 2 cm test section
- Equipped with pressure ports and Pitot ports
- Ceramic/copper pulsed and DC electrode blocks
- Stagnation pressure $P_0=0.2-1.0$ atm
- Ionization: repetitively pulsed discharge
Laser Differential Interferometry (LDI) diagnostics: BL density fluctuation spectra measurements

Diagram showing the experimental setup with various components labeled:
- Mirror
- Flow
- Magnet pole
- Magnet coil
- He-Ne laser
- Photodiode
- Reference beam
- Probe beam
- Flow direction

The diagram includes optical components such as Wollaston prisms, quarter-wave plates, convex lenses, and a test section.
Boundary layer visualization by laser sheet scattering: comparison with a 3-D compressible Navier-Stokes flow code

P₀=150 torr, 2 mm from the wall

P₀=250 torr, 2 mm from the wall

P₀=150 torr, 2 mm from the wall
Repetitively pulsed discharge (40 kHz rep rate) + DC sustainer in M=4 air flow

Air, M=4, B=1.5 T

$P_0=1\ \text{atm}, \ P_{\text{test}}=13\ \text{torr}, \ U_{\text{max}}=13\ \text{kV}$

Plasma always remains uniform and stable for run times of several seconds

Shock train in a M=3 low-pressure diffuser

How did we achieve that?
Pulser-sustainer discharge: stable plasmas at high powers
M=3 nitrogen flow, P₀=1/3 atm, Pₜₐₜₐₜₜ = 8 torr

Voltage [kV]

Current [A]

Pulse energy 1-2 mJ
Time averaged pulsed discharge power 40-80 W

<σ> = 0.073 mho/m, B = 1.5 T

<Î> = 0.9 A
DC discharge power 1.4 kW
MHD effect on boundary layer density fluctuations: Accelerating vs. retarding Lorentz force

Decelerating force

Accelerating force

Air, \( M=3 \), \( P_0=250 \) torr

Boundary layer fluctuations increase by retarding Lorentz force
Flow acceleration / deceleration by MHD:
Static pressure measurements in M=3 air flows

Air, $P_0=250$ torr, $P_{test}=8.7$ torr
$U_{PS}=2$ kV, $R=0.5$ kΩ, $<I>=1.2$ A
Pulsed discharge duration 0.5 s

\[
\frac{\Delta p_R - \Delta p_A}{p} = 0.11
\]

Joule heating factor:
\[
\alpha=0.10
\]
(90% of discharge energy stored in $N_2$ vibrations)
Comparison with quasi-1-D theory

\[ \Delta M_\pm = -0.13 \text{ at } I = \pm 1.0 \text{ A in air} \]

\[ \Delta p_R - \Delta p_A \approx 2 \cdot \frac{(\gamma - 1)M^2 + 1}{M^2 - 1} \cdot j_y B_z L \]

Very good agreement with experiment
Comparison with 3-D Navier-Stokes code: velocity and pressure profiles

Predicted velocity change $\Delta u = 14$ m/sec (2%)
Further insight: Molecular Tagging Velocimetry (MTV) in NO-seeded MHD flows

1% NO in N₂

Images of “painted” line at t=0 ns and t=600 ns

Fluorescence
\( \text{NO}(A^{2}\Sigma) \rightarrow \text{NO}(X^{2}\Pi) \)

Cold flow velocity: \(647 \pm 4 \text{ m/s}\)

3-D Navier-Stokes code prediction: \(660 \text{ m/s}\)

Flow velocity with plasma/MHD on: \(471 \pm 9 \text{ m/s}\)

Much slower than predicted by code (evidence of stronger Joule heating?)
Case 3: Electric Discharge Excited Oxygen-Iodine Laser ($\lambda=1.3$ $\mu$m, c.w. power 1.5 W)

Discharge volume 50 cm$^3$, pressures up to 460 torr, flow rate up to 0.1 mole/sec (O$_2$), 1 mole/sec (He)
Crossed pulser-sustainer discharge characterization: 10% O₂ in He, P₀ = 120 torr

**FID pulser:**
40 kV peak voltage, 5 ns pulse duration, 100 kHz pulse rep rate, duty cycle <1/2,000

**Sustainer discharge voltage and current**
Crossed pulser-sustainer discharge: targeted energy loading (controlled by $T_e$, or $E/N$)

10% O$_2$ in He:
up to 30% of input power goes to O$_2$(a$^1\Delta$) state
Discharge Excited Oxygen-Iodine Laser (DOIL) Kinetics

\[ O_2 (X^3\Sigma) + e \rightarrow O_2 (a^1\Delta) + e \]

\[ n \cdot O_2 (a^1\Delta) + I_2 \rightarrow n \cdot O_2 (X^3\Sigma) + I + I \]

\[ O_2 (a^1\Delta) + I \leftrightarrow O_2 (X^3\Sigma) + I^* \]

\[ I^* \rightarrow I + h\nu \]

Need as much \( O_2 (a^1\Delta) \) as can be produced

Need low temperature to shift equilibrium in reaction (3) to the right (i.e. more \( I^* \))
Singlet delta oxygen yield measurements by emission spectroscopy *(radiative lifetime 75 min)*

The Ohio State University

<table>
<thead>
<tr>
<th>$P_0$, torr</th>
<th>Discharge power, kW</th>
<th>$P$, torr</th>
<th>M</th>
<th>T, K</th>
<th>SDO yield, %</th>
<th>Threshold yield, %</th>
<th>Power stored in SDO, W</th>
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</thead>
<tbody>
<tr>
<td>60</td>
<td>1.6</td>
<td>1.9</td>
<td>3.0</td>
<td>120±15</td>
<td>5.7±0.85</td>
<td>2.3</td>
<td>110</td>
</tr>
<tr>
<td>120</td>
<td>2.1</td>
<td>3.8</td>
<td>3.0</td>
<td>120±15</td>
<td>5.0±0.75</td>
<td>2.3</td>
<td>200</td>
</tr>
</tbody>
</table>

Intensity (arbitrary units)

Yield, %

Discharge power, kW
Case 4: Low-temperature plasma assisted combustion
Ignition in C$_2$H$_4$/air: P=70 torr, u=15 m/s, $\Phi=0.9$, $\nu=40$ kHz

- N$_2$ emission: plasma temperature
- CH emission: flame temperature
- Flow direction
Plasma temperature: $N_2$ visible emission spectra
Species concentrations: FTIR absorption spectra

Plasma temperature: $N_2$ visible emission spectra
Species concentrations: FTIR absorption spectra
Ethylene/air: different flow velocities

P=70 torr, Φ=1.0, ν=50 kHz

Significant fuel oxidation, resultant flow temperature rise

Kinetic analysis suggests that pulsed discharge generates significant amounts of O atoms (chemically active radicals)
Nonequilibrium air flow characterization:
What species do we need to measure?
How are we going to generate them?

\[
\text{N}_2(\text{electronically excited}) + \text{O}_2 \rightarrow \text{N}_2 + \text{O} + \text{O}
\]

\[
\text{O}_2(\text{electronically excited}) \rightarrow \text{O} + \text{O}
\]

\[
\text{N}_2(v), \text{O}_2(v), \text{O}_2(a^1\Delta), \text{O}, \text{and NO}
\]

Pulser-sustainer discharge operated at different E/N
How are we going to measure these species?

**Air species vibrational level population measurement:**
**Spontaneous Raman spectroscopy**

- Uses CO laser (up to 50% efficiency), scalable to high powers
- Based on resonance absorption of laser radiation by CO molecules
- V-T losses are small ⇒ Energy remains locked in molecular vibrational modes
- Works at high pressures (P>1 atm), low temperatures (T~500 K), modest power densities (~100 W/cm²),
Optical pumping of air with a CO laser

Dual CO laser system

Absorption cell

Optically pumped plasma
Schematic of Raman spectroscopy measurements

Species: CO, NO, CO₂
Species: CO, N₂, O₂
Spatially resolved Raman spectra of N$_2$, CO, and O$_2$ at 1 atm

CO/N$_2$/O$_2$=5/75/20, P=1 atm
(laser power 10 W)

Spatial resolution 250 $\mu$m
Vibrational temperatures and level populations of N$_2$, CO, and O$_2$ at 1 atm

Vibrational temperatures: 2000-3000 K, rotational temperature: 300 K

Good agreement with master equation modeling
Raman spectra and vibrational level populations of N$_2$, CO, and O$_2$ at 0.5 atm

CO/N$_2$/O$_2$=8/88/4, P=0.5 atm (laser power 10 W)

5 vibrational levels of N$_2$, 16 vibrational levels of O$_2$

Good agreement with master equation modeling
Schematic of pulsed Raman pumping of $\text{N}_2$ (w/o CO laser)

Pump Nd:YAG laser operates at 10 Hz
Stokes signal generated in a high-pressure Raman cell
Pulsed Raman pumping: time-resolved vibrational level populations of $\text{N}_2$

"Instantaneous" $v=1$ pumping (single pump laser pulse $\sim 10$ nsec)

Time resolution $\sim 0.1$ µsec, spatial resolution $\sim 100$ µm

Rates of vibration-vibration energy exchange for $\text{N}_2$-$\text{N}_2$ inferred from level populations
Pulsed Raman pumping: time-resolved vibrational level populations of O₂

Relaxation Rate Constant, cm³/s

Rates of vibration-vibration energy exchange for O₂-O₂ inferred from level populations
O atom concentration measurements:
Two-Photon Absorption Laser Induced Fluorescence (TALIF)
with Xenon Calibration

Measuring ratio of spectrally integrated O atom TALIF signal to that of xenon with identical laser beams, signal collection optics, spectral filtering and PMT gain

Relative signal converted to absolute O atom number density

Estimated combined uncertainty of absolute O atom density about 40%
O atom number density after a single high-voltage nanosecond discharge pulse: TALIF measurements

Peak O atom density in air: $0.9 \cdot 10^{14}$ cm$^{-3}$/pulse, decay time: 2 msec

Kinetic model correctly predicts O atom densities and decay rates in all three cases
TALIF O atom number density measurements after a burst of high-voltage pulses

Air, methane-air, and ethylene-air mixtures, $P=60$ torr, $\Phi=1.0$, pulse burst (up to 100 pulses/msec)

Significant O atom accumulation after 100 pulses in air: 0.2%

Half of input pulse energy goes to oxygen dissociation
How are we going to predict effect of these species on the flow?

- Applicable for non-collinear collisions of rotating molecules
- Applicable in a wide range of gas temperatures ($T \sim 300-10,000$ K)
- Excellent agreement with 3-D computer calculations
- Fully analytic
Rate models applicable up to very high temperatures
Model validation:
NO IR and UV emission behind strong shocks

NO emission profiles behind the normal shock in air. \( P_0 = 2.25 \) torr

- NO IR emission behind strong shocks
  - \( u_s = 3.85 \) km/sec
  - \( u_s = 3.78 \) km/sec

- IR emission
  - \( u_s = 3.85 \) km/sec

- UV emission
  - \( u_s = 3.78 \) km/sec
Effect of vibrational relaxation on shock standoff distance: quite noticeable

Nitrogen, $M=4$, $T=300$ K, $T_v=3000$ K, $P=10$ torr, nose radius 5 mm

With and without 1% of water vapor

Stand-off distances increases from 0.9 to 1.3 mm
New Research Program: Effect of Excited Species ($N_2(v)$, $O_2(v)$, O atoms, and $O_2(a^1\Delta)$) on M=5 Flow Field

Stagnation enthalpy: 0.3–0.6 MJ/kg

Steady-state flow (~ 10 sec)

LENS: 10-15 MJ/kg

Run time ~ 1 msec
Objectives

• Stable, high-pressure, nanosecond pulser – DC sustainer discharge in nozzle plenum ($P_0 \sim 1$ atm)

• Flows: air, $N_2$/He, $O_2$/He, $N_2$/Ar, and $O_2$/Ar

• Varying DC voltage ($E/N$): targeted energy loading into $O_2(a^{1}\Delta)$ ($E/N=5$-$10$ Td), $N_2(v)$, $O_2(v)$ (10-$50$ Td), and O atoms (100-$200$ Td, no DC)

• $M=5$ flow in supersonic test section ($P \sim 1$ torr)

• Blunt body in test section (D$\sim$5 mm), shock stand-off distance $\sim 1$ mm

• Schlieren and plasma shock visualization; shock stand-off distance measurements with and without excited species present

• First spatially resolved measurements of rotational temperature, $O_2(a^{1}\Delta)$, $N_2(v)$, $O_2(v)$, and O atoms behind the $M=5$ bow shock: IR emission, spontaneous Raman, CARS, TALIF ($\sim100$ $\mu$m resolution)
Objectives (continued)

• Strong vibrational excitation of \( \text{N}_2, \text{O}_2, \) and \( \text{H}_2 \) using a pulse-burst laser for Raman pumping (20-30 pulses at 1 pulse/\( \mu \)sec rep rate). Measuring vibrationally induced dissociation at high energy loading (several vibrational quanta per molecule) using TALIF

• Comparison with coupled compressible Navier-Stokes / master equation modeling and rate model validation: state-specific vibrational energy transfer and dissociation rates, rates of \( \text{NO} \) production, \( \text{O}_2(a^1\Delta) \) quenching rates

• Developing instrumentation for using at LENS hypersonic flow facility

• Developing physics-based design tool nonequilibrium flow models with predictive capabilities
Other Future Research Thrusts in High-Speed Propulsion and Power

- Confident ignition / flameholding / relight in high-speed flows (using large-volume nonequilibrium plasmas)

- Demonstrating scaling potential of DOIL laser power to make The Application feasible: tens to hundreds of W in a laboratory scale setup

- MHD: electrical power generation in reentry flows, opening up “transmission windows” through reentry plasma using B field, power generation in scramjets (stagnation temperature too high for a turbine)
Plasma assisted ignition / flameholding in high-speed flows

- Fuel injection cavity filled with plasma
- Optical access windows
- High voltage pulse electrode
- Straight channel or nozzle inserts
- Flow
DOIL Laser Scaling