Advanced Kinetic-Based Modeling Applied to Plasma and Neutral Flows

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AFRL Research and Collaborations

- FRC thruster modeling
  - MSNW
  - Dr. David Kirtley

- Optical lattices for gas heating and gas-surface interactions
  - AFOSR/Physics (RSE)
  - Dr. Tatjana Curcic

- Radiometric forces for near-space vehicle propulsion
  - AFRL/RQRS
  - Advanced Concepts Group
  - Dr. Marcus Young

- New approaches to nonequilibrium flows
  - AFRL/RQAC
  - Computational Sciences Branch
  - Dr. Eswar Josyula

C – Computational  E – Experimental  Black – Funded by AFOSR/RSA  Red – Funded elsewhere
Energy Deposition in Gases from Pulsed Optical Lattices, CRS & CRBS Diagnostics

**High intensity:** expected to drastically increase gas temperatures, thus enabling unprecedented analysis of thermal and chemical rates and cross sections

**Low intensity:** CRS and CRBS, unique non-intrusive all-in-one diagnostics of macro- and micro gas properties at micro-scale

Counter propagating pulses with same path length
Probe laser separate from pump lase, I and p varied

Experiment and computation agree

Gas temperature effect demonstrated

Experimental and numerical analysis
High-Altitude Airbreathing Propulsion: Fundamentals of Radiometric Flows

- Use of available atmosphere and sun-generated temperature gradients
- Altitude 40-60 km, Pressure $\approx 4 \times 10^{-4}$ atm, $\lambda_{mfp} \approx 200 \ \mu m$

Fundamental research stems from work of Maxwell, Reynolds, Einstein

- Demonstrated innovative approach--momentum accommodation
- Combined experiments and modeling of radiometric flows
- Accommodation coefficients obtained for three gases; validated on existing data
- Negative thermophoresis experimentally confirmed

Highly accurate torsion balance
Flexural Pivots
Electrostatic Calibration Combs
LVDT
Radiometer

High accuracy experimental data sets are obtained

- Sources of radiometric forces clarified
- Impact of chamber walls characterized
- Multi-vane geometries studied

Highly accurate torsion balance
Flexural Pivots
Electrostatic Calibration Combs
LVDT
Radiometer

Significant (in theory, up to 100 times) increase in force
FY12 Publications


- About 15 refereed conference presentations/papers (AIAA conferences and RGD Symposium)
FRC Thrusters: Features and Challenges

What is an FRC?
Derived from fusion technology
- Efficient plasma formation
- Gas independent (Air, Ar, Xe, Ne)

Cylindrical coil surrounding insulated discharge chamber
High speed transient B field generates azimuthal E field
Neutral gas injected into discharge chamber ionizes
Plasma is supersonically accelerated inward creating compression and heating (further ionization)

Toroidal plasma confinement
Plasma induces current which generates a magnetic field in opposite direction of applied field
Extreme pressure tends to drive plasma out of discharge chamber

Difficulties in modeling FRCs
High density, MHD plasma
High temperature, $T_e \sim 10 - 1000$ eV
Non-equilibrium
Chemical (Air) / Ionization mechanisms
Neutral gas entrainment

MSNW FRC thruster
Current Status

- can be translated and accelerated to provide thrust by applying a gradient of magnetic pressure using pulsed external coils
- operates at a temperature that is optimal for ionization
- well confined

- Basic concept of operations has been demonstrated (Kirtley, Brown, and Gallimore 2005)
- Further optimization of the formation process (Miller, Rovey 2009)
- One of the latest design iterations (Slough, Kirtley, and Weber 2009) provides plasma velocities in the 10-40 km/sec range, a desirable regime for USAF applications
- Power and mass utilization efficiencies TBD more precisely
- Thrust augmentation is still desired (dual mode)

Since the plasma density in the FRC is close to optimal \( b \approx 1 \), the latter could be achieved in two ways:

1. increasing the molecular mass of the propellant
2. increasing the effective mass by gas entrainment
Neutral Entrainment

(1) the easiest to achieve: xenon, the largest mass of any (stable) noble gas could be an ideal candidate
Problems: a high-Z plasma has higher rates of radiative and collisional (effective ionization cost) energy losses, thus reducing the efficiency + reaction related caveats

(2) tentatively more attractive but more difficult to achieve
★ Neutral entrainment (Cambier 2006): FRC plasmoid propagates into ambient gas and captures or pushes it while being accelerated by the external coils
★ In this fashion, the system is able to exert a force on a composite object with a higher mass, while the plasma itself is kept at optimal physical conditions for high efficiency
• Dynamics of the entrainment, momentum coupling and mixing processes at the FRC/gas interface are critical to the efficiency
• Kirtley, Slough et al (2011): first experimental proof of concept
• Charge exchange reactions
Short-Term Objectives

- Numerically study the process of neutral entrainment of an FRC plasmoid
- Main focus: analysis of the relative importance of the electron impact ionization and charge exchange reactions between the neutral and charged particles

I. the balance between ionization and charge exchange reaction rates is examined for various gases and temperatures

II. a study of heat bath relaxation is performed and the impact of Coulomb collisions is clarified

III. Celeste3D particle-in-cell computational tool, extended to include the interactions between the charged and neutral particles and neutral particle transport, as well as Coulomb interactions between charged particles, is used in simulations of an FRC plasmoid and neutral gas interaction
Neutral Entrainment: Reaction Rates

- Electron impact ionization (EII, $A+e \rightarrow A^++e+e$): SIGLO database provides cross sections; rates are calculated as
  \[
  k_{eii} = \int g\sigma_{eii}(g)f_e(g)\,dg
  \]

- Single charge exchange (SCX, $A+A^+ \rightarrow A^++A$): expressions from Losev et al (2002) are used for the cross sections, integrated as in EII
  \[
  \sigma_{scx} = \begin{cases} 
  0.5\pi a_0^2 \frac{Ry}{E_i} \log^2 \left(100\sqrt{\frac{E_i}{\epsilon} \frac{\mu}{m_e}}\right) & \epsilon \geq \epsilon^* \\
  \pi \sqrt{\alpha e^2/2\epsilon} & \epsilon < \epsilon^*
  \end{cases}
  \]
  \[
  \epsilon^* = \frac{2\alpha e^2}{a_0^4} \frac{E_i^2}{Ry^2} \left(\log \left(100\sqrt{\frac{E_i}{\epsilon^*} \frac{\mu}{m_e}}\right)\right)^{-4}
  \]

- Recombination reactions that include three-body recombination and radiative photorecombination ($A^++e \rightarrow A+h\nu$) taken from Raizer (1991)
Recombination is not important

Ionization reaction rate is lower than charge exchange rate: may point to efficiency of entrainment

$T < 10\text{eV}$ a typical entrainment time of 50ms, the fraction of ions that participate in charge exchange may be as low as 10% when neutral density $< 10^{18}\text{m}^{-3}$

Higher neutral density may be required

Nitrogen: air breathing potential

Recombination rate (dissociative recombination is included) dominates at $T < 5\text{eV}$

EII dominates at $T > 5\text{eV}$

May create problems for entrainment
Reaction Rates, cont'd

Xenon

- Xe: high thrust
- Ionization energy low, thus EII rate is about two orders of magnitude larger than SCX
- Efficiency of may suffer

Neon

- Neon: high ionization energy
- Recombination (not shown) is not important
- SCX rate higher than EII, thus efficiency may be high
- Selected for further study
Adiabatic Relaxation of Neon Plasma

- **Entrainment**: cold stagnant neutral atoms collide with the fast moving plasma ions and electrons.

- Relaxation process depends on many factors such as plasma temperature, concentration of reacting species and the relationship between different reaction rates.

- Consider the effect of these factors on the time evolution of plasma and neutral properties in **adiabatic heat bath**.

- Initially the neutral species and the charged species have relative velocity $U$ (used 20 km/s and 30 km/s).

- Initial plasma temperature 10 eV, the neutral temperature is 300 K, and both neutral and plasma density are $10^{18} \text{m}^{-3}$.
Energy of relative motion is converted into thermal, and T of heavy species increases.

Thermal relaxation of electrons on neutrals and ions is fairly slow.

Change in $T_e$ is primarily related to the electron impact ionization reactions.

Impact of U on electron temperature becomes visible only after 100 $\mu$s.

For any U and T, there is a strong thermal non-equilibrium.

$\eta_i$ weakly depends on U.

Electron T is very important.

Number of charge exchange reactions for $T=10$ eV and $U=20$ km/s was found to linearly increase with neutral density.

The dependence of the number of ionization reactions on neutral density is weaker than linear.

Further increase slowed by the depletion of high energy electrons.
Goal: develop a computational capability capable of accurate modeling of FRC neutral entrainment at kinetic level

- Celeste3D developed by J. Brackbill at Los Alamos selected as the main production and development tool: 3D PIC that solves the full set of Boltzmann-Vlasov eqns
- Benefits: kinetic (PIC based and thus amenable to DSMC-like neutral addition), implicit (large time steps allow modeling of neutral entrainment), full 3D
- Physical challenges: plasmoid formation & translation, neutral capability addition, open boundary conditions, many physical and chemical processes
- Numerical challenges: multi-processor domain decomposition parallelization, adding flexible initial conditions and non-rectangular geometries

Progress:
- Neutral entrainment modules
- Arbitrary initial condition capability
- Plasmoid / neutral interaction
- Open boundary conditions
Modified Celeste3D

- Extended to include neutral transport and collisional relaxation.

- Particle-based kinetic capability includes the following collisional processes:
  - neutral-neutral collisions (VHS model)
  - charge exchange reactions (Losev's cross sections)
  - neutral-ion elastic collisions (according to Losev)
  - the electron impact ionization (SIGLO)

- Hard sphere after-collision scattering is assumed for all these processes, with the exception of charge exchange reactions, for which the velocities of neutrals and ions are swapped.

- Species weighting scheme is implemented.

- Majorant collision frequency scheme in spatial cells.

- Coulomb collision module has been added to Celeste, based on a particle-weights scheme of Nanbu.
2D (planar) flow, 40 by 80 grid

Initial conditions: Schmid-Burgk equilibrium with \( n_p = 10^{18} \text{m}^{-3} \) and \( T_p \) of 5 and 10eV

Number of simulated ions, electrons, and neutrals per cell: 64, 100, and 512

Weighted electron mass, \( m_i/m'_e = 100 \)

Reference frame of the plasmoid: neutral gas injected into the computational domain from the left boundary

Neutral gas properties changed to study their impact on the neutral-plasma interaction

Periodic (10eV plasmoid) and open (5eV plasmoid) BC for plasma and open BC for neutrals at left and right boundaries

Specular conducting wall at top and bottom boundaries

No neutrals test runs: equilibrium is maintained for at least 10,000 ion plasma periods (over 30\( \mu \)s)
At 16μs, neutrals loss near the centerline amounts to about 30%.
Loss of neutrals = gain in ions.

8ms: impact of neutrals is negligible
12ms: moderate, on the order of 5%, increase in plasma density in the center
16ms: plasma density in the center decreases due to mass transfer
Significant elongation of the plasmoid
Baseline: modest (~5%) increase in \( n_i \)
- Clear translation of the plasmoid
- Average velocity of initially stationary plasmoid is about 3 km/s
- U=30 km/s: weaker interaction (short t)
- Larger n: \( p \) transfer, ionization triple

Neutral density decreases by ~50% for the baseline and ~30% for U=30 km/s
- Since change in \( n_i \) is < change in \( n_n \), the latter is related to charge exchange
- Neutrals lose X momentum after charge exchange, and do not reach right boundary
Summary

First step toward accurate modeling of FRC thruster with neutral entrainment

Comparison of ionization and charge exchange reaction rates indicates that the use of nitrogen and especially xenon may be problematic, while neon appears to be a fairly good propellant

Adiabatic heat bath:
- showed that FRC entrainment proceeds under conditions of strong thermal and chemical non-equilibrium; ion, electron, and neutral temperatures strongly differ, and the electron distribution function is non-Maxwellian
- Strong impact of electron temperature on plasma density due to ionization
- Modeling of Coulomb collisions between electrons is desirable to properly account for electron high velocity tail depletion

2D modeling:
- Implicit PIC code Celeste3D extended to include neutral transport, plasma-neutral and neutral-neutral collisions and Coulomb collisions
- For 5eV and 10eV, strong entrainment of neutral particles by a translated plasmoid is observed as a result of charge exchange reactions between slow neutrals and fast moving ions
- Modest increase in plasma density due to electron impact ionization
- Increase in neutral density appears highly beneficial for thruster efficiency
Outlook

Future directions in kinetic modeling of FRC thrusters:

- Electronic excitation
- Air breathing
- 3D and annular configurations
- RMF, plasmoid formation
- Parallelization
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