DEVELOPING NUMERICAL SIMULATIONS TO ASSIST IN ISOLATING EXCITED NITROUS OXIDE STATES

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20th Advanced Space Propulsion Workshop (ASPW2014) Ohio Aerospace Institute, Cleveland, Ohio, November 17-19, 2014

Outline

- Introduction
- Experimental
  - System Design
  - Results
- Computational Analysis
  - Motivation
  - Current Work
- Future Work

Introduction

Overview

- Purpose
  - Demonstrate dissociation of nitrous oxide with non-thermal plasma discharge
- Final objective
  - Achieve self-sustained dissociation using a dielectric barrier discharge (DBD)
  - Design and fabricate a hybrid electric/monopropellant thruster with this technology
- Nitrous oxide dissociation
  - **$N_2O(g) \rightarrow N_2(g) + \frac{1}{2}O_2(g)$ + Heat**
    - 161 kJ/mol required to break apart N_2O
    - Oxygen molecules recombine and release 245 kJ/mol
    - Net energy ~ 84 kJ/mol
  - Self-sustained dissociation can be reached at high temperatures (>1000 °C)
- Benefits
  - "Greener" propellant than current monoprop's (hydrazine, hydrogen peroxide)
  - Comparable specific impulse (~200 sec)
  - Non-toxic/non-flammable, safe to handle
  - Can be stored as a liquid

Past Research

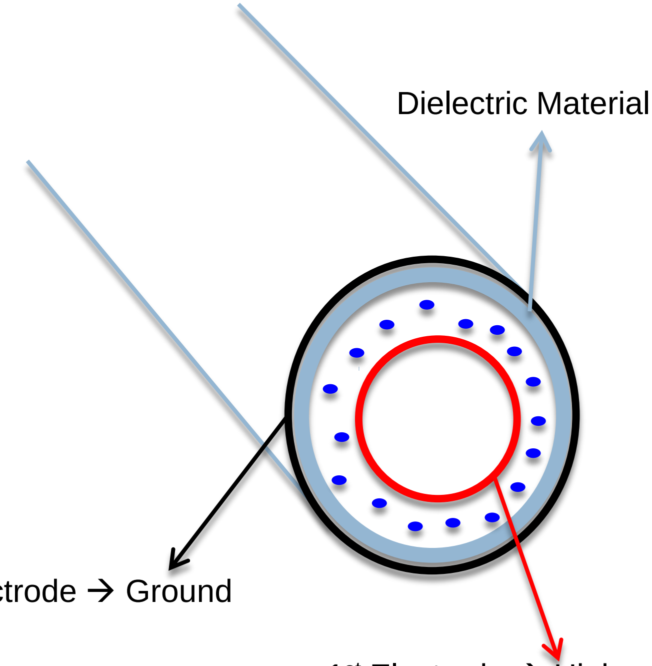
- Previous Experiments
  - Catalysts
    - Reduce dissociation temperature
    - Power only required at startup
    - Material limitations
      - Not stable at high temperature
  - Plasma
    - Dissociation of NO_X
    - Increased rate of decomposition
    - 100% conversion achieved
    - Continuous external power required

Hypothesis: Due to some of the gas being in an excited state, the effective activation energy for dissociation due to collisions may be reduced

Experimental: System Design

Dielectric Barrier Discharge

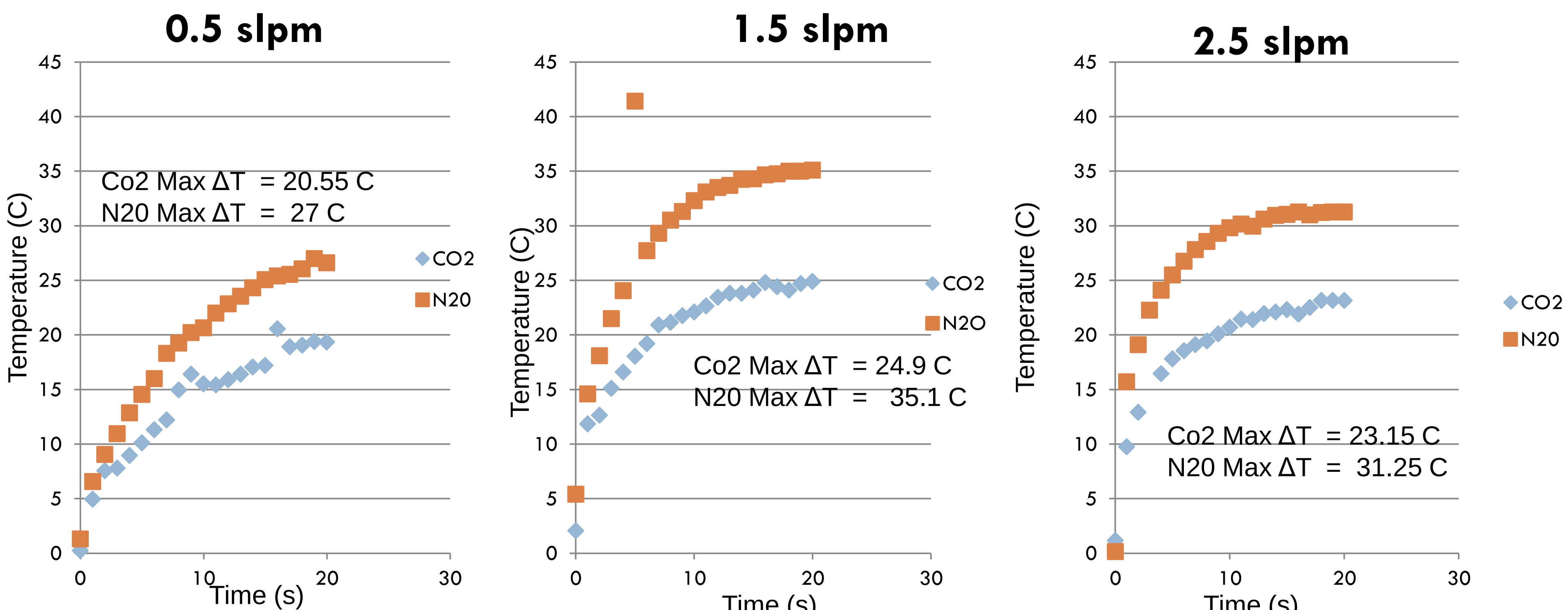
- Dielectric Barrier Discharge (DBD)
  - Two concentric electrodes separated by an insulating dielectric barrier
  - High voltage AC
- Varying electric potential to accelerate free electrons
  - Electrons then collide with N_2O
  - Ions/additional free electrons formed
  - Trapped ions enhance collisionality
  - Only excitation and not full ionization may be sufficient
    - Reduction in activation energy predicted



Proof of Concept Results

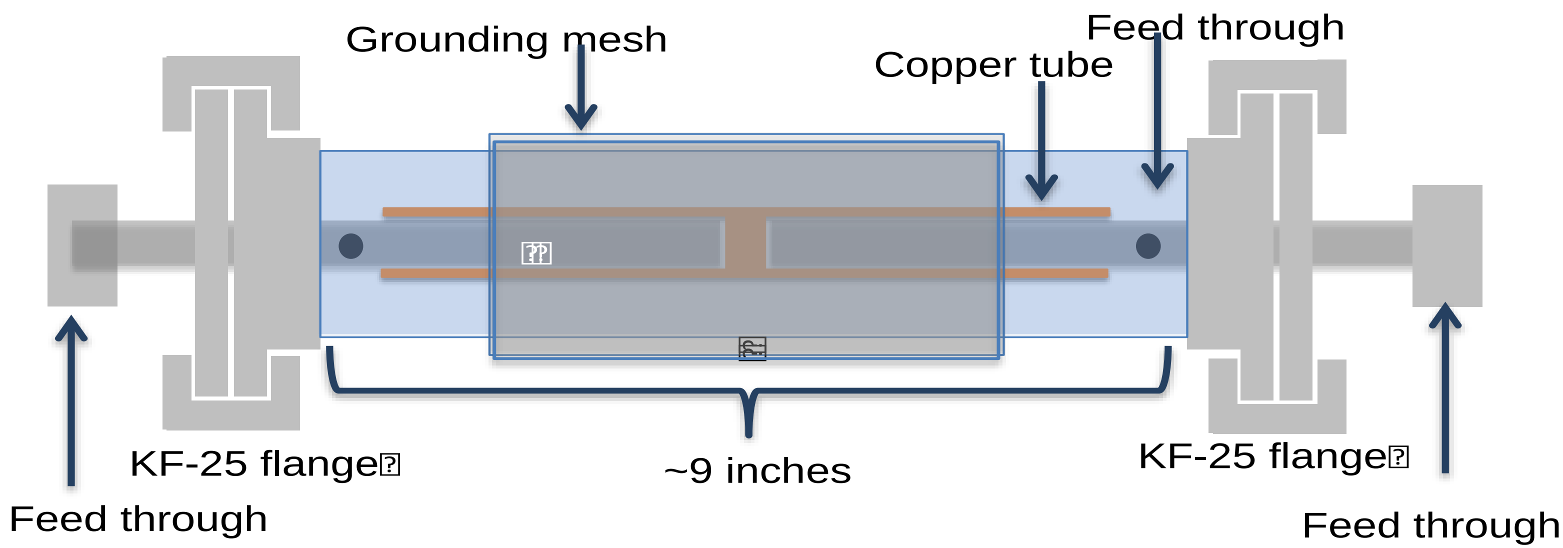
EXPERIMENTAL

- Tests using CO_2 as a control
- The specific heat for CO_2 is about 5% lower than N_2O.
  - This would result in CO_2 having a higher temperature increase (only joule heating)
  - However, we see the exact opposite



Current Design

EXPERIMENTAL

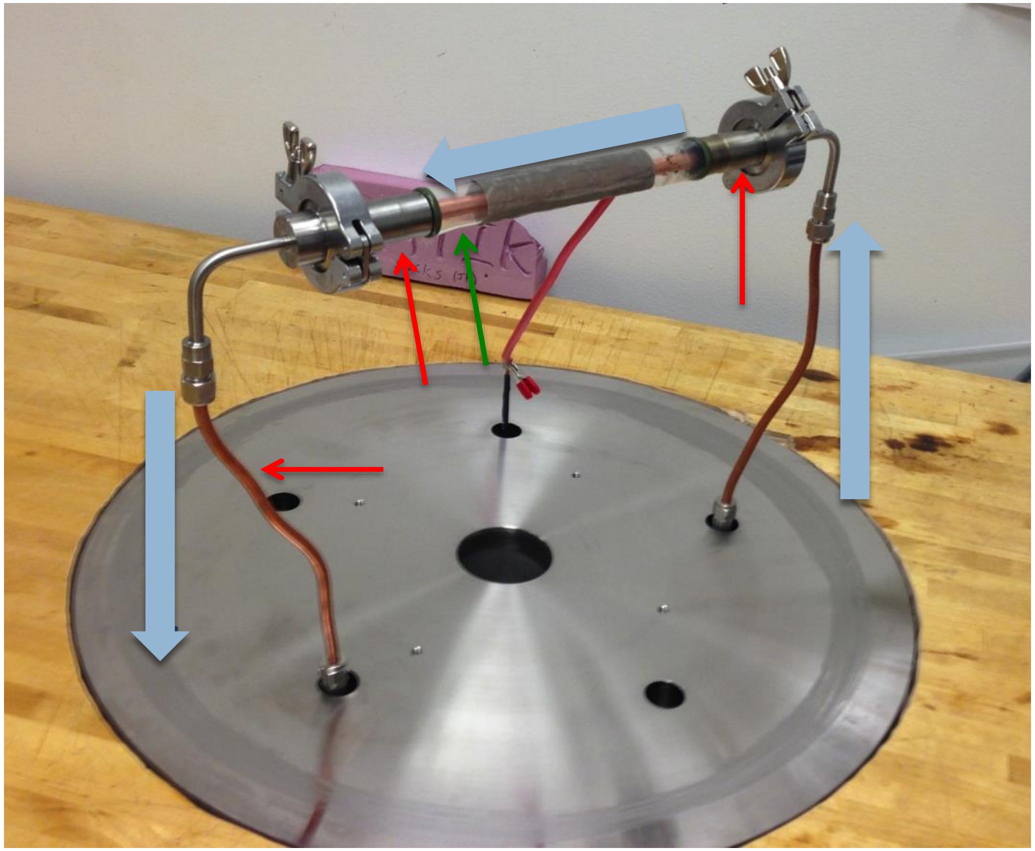


- Fused two stainless steel to quartz adapters (KF 25 Flanges)
- Placed in Bell Jar
  - Feed-throughs were connected to KF-25 ports on plate
  - Copper tube will “hold” the two feed-throughs
    - Direct flow out/in the holes in the feed-throughs
- Entire system grounded to grounding mesh

Bell Jar and Instrumentation

EXPERIMENTAL

- External flow meter
  - Switch between CO_2 and N_2O
  - Blue arrows show flow direction
- Thermocouples
  - Shown with red/green arrows
  - Red arrows are surface mounted to flanges and exit flow tube
  - Green arrow is internal to flow immediately downstream of plasma region
- Power input
  - *High voltage probe
  - *Series resistor to measure current



Reactor shown mounted on base plate without bell jar

*Some challenges still need to be addressed

Characterizing Power Loss

EXPERIMENTAL

- Power can be divided into the following:
  - Input power from plasma driver
    - Measured
  - Decomposition power
    - Unknown
  - Enthalpy increase of gas
    - Calculated using specific heats/tabulated values and measured temperatures
  - Radiative power loss
    - Inferred → will be baselined using CO_2

$$P_{input} + P_{decomp} - P_{rad} = P_{enthalpy}$$

Experimental: Results

Results

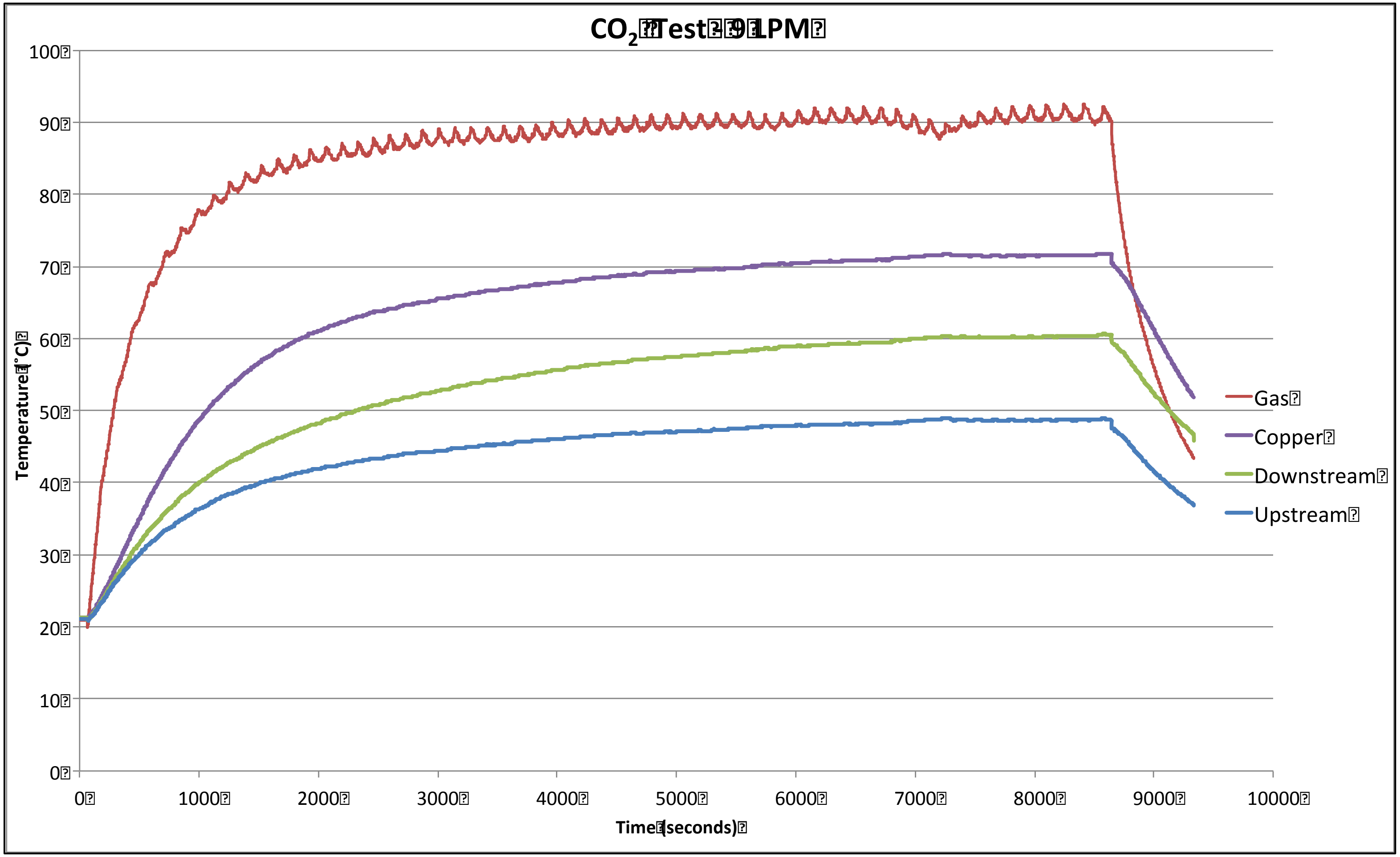
EXPERIMENTAL

- Results with latest design
  - Gas flow at 9 LPM, ~30% maximum voltage
  - Run for about 2 hours to ensure steady-state
- Temperature data recorded from all four thermocouples
- Oscillation in gas temperatures
  - Period of ~2.5 min
  - Correlation to oscillation in the flow rate
  - Inverse relation shows higher temps at lower flow rates
    - Relationship is as expected, but cause of oscillation is currently unknown

CO_2 Temperature Data

EXPERIMENTAL

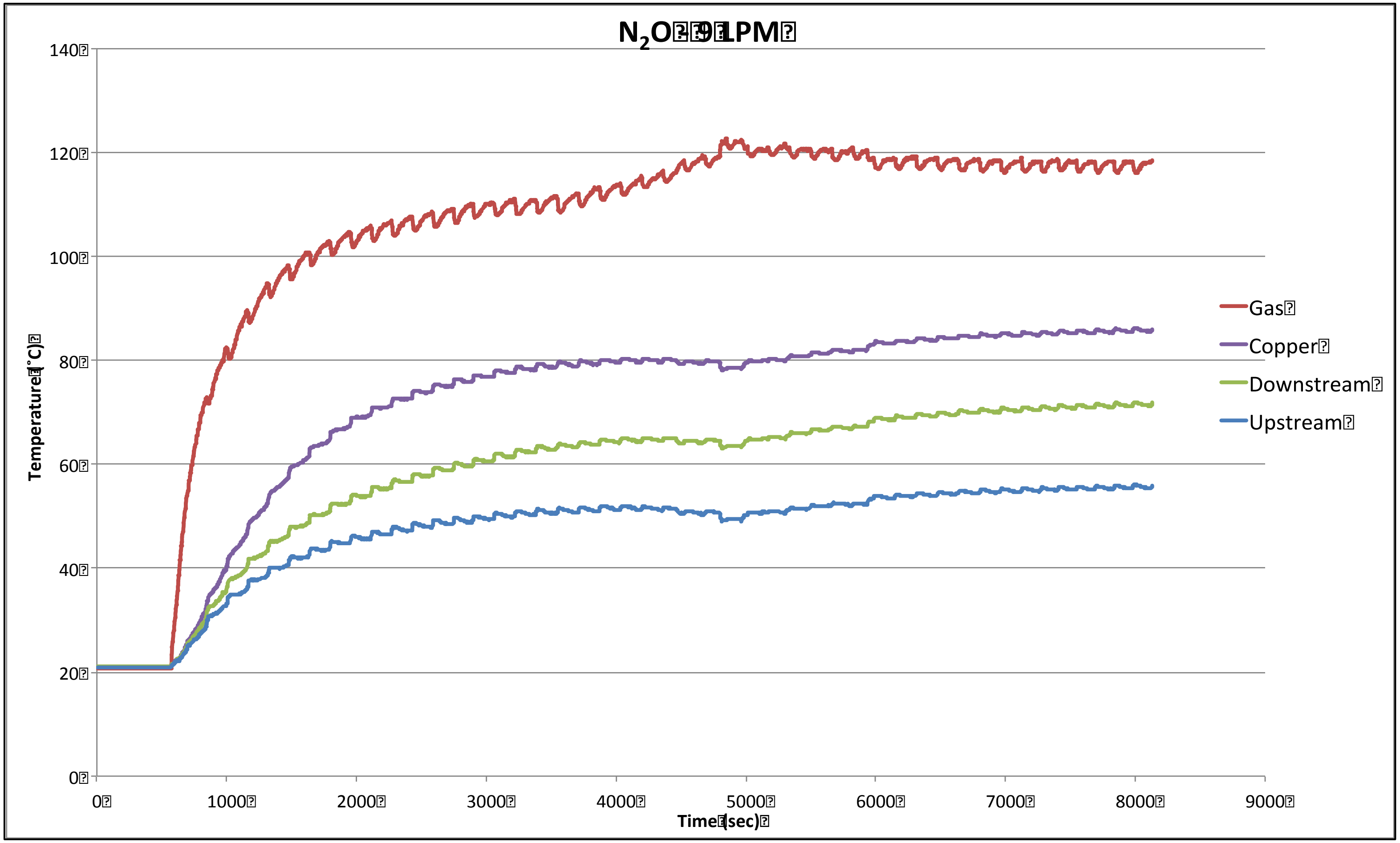
- Peak gas temperature around 90˚C



N_2O Temperature Data

EXPERIMENTAL

- Peak gas temperature around 120˚C



Data Analysis: N_2O versus CO_2

EXPERIMENTAL

Location	% Power Increase
Power Supply	31
Gas (Enthalpy)	37
Copper (Rad)	17
Downstream (Rad)	15
Upstream (Rad)	7

6% difference

- Graphs show temperature is higher (30˚C) for N_2O
- ~31% more power into the N_2O from the power supply
  - Characteristic of ionization/excitation energies and cross-sections
- Radiated power increase shown above at each thermocouple location
- Conclusion
  - Net power released through decomposition of N_2O
  - Presence of plasma is either:
    - Reducing activation energy (low energy cost – desirable) or
    - Directly dissociating N_2O (high energy cost – not desirable)

Computational Analysis: Motivation

Isolating Excited States of N_2O

COMPUTATIONAL

- External power required to dissociate N_2O is deemed excessive
  - High energy cost – not desirable
- Hypothesis:
  - Due to some of the gas being in an excited state, the effective activation energy for dissociation due to collisions may be reduced
- Ionization energy for N_2O – electrons accelerated in DBD
  - ~12.9 eV
- Goal: Input energy less than that to minimize the amount of power required

Dissociation Paths

COMPUTATIONAL

- Possible dissociation paths with energies less than ~ 13 eV
  - 7.8 eV
  - 8.5 eV
  - 9.6 eV
- Build/design an electron source
  - Accelerate electrons to certain energy levels
  - Collide with neutral gas, induce excitation

Computational Analysis: Current Work

Numerical Model

COMPUTATIONAL

- A 2-D numerical model will provide a guideline for experimentation
- First step → 1-D model of plasma within a chamber
  - Implement "extractor grids" to accelerate electrons
- Simulation (1-D):
  - Fluid treatment for ions and electrons
  - Transport model: Drift Diffusion
    - Drift – electric field, Diffusion – gradient of density, temperature

Scharfetter-Gummel (SG) Method

- Method used to discretize the drift-diffusion equations
- Species density evaluated on cell centers (*i*)
  - All other quantities evaluated on cell boundaries ($i \pm 1/2$)
- Fluxes approximated across the cell
  - All variables constant other than density
  - First order differential equation in density
  - Provides more stability

Equations (1)

COMPUTATIONAL

Electrons	Ions

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = S_e$$

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \Gamma_i = S_i$$

$$\Gamma_e = -\mu_e E n_e - \mu_e T_e \nabla n_e - k_t \mu_e n_e \nabla T_e$$

$$\Gamma_i = \mu_i E n_i - \mu_i T_i \nabla n_i$$

Assuming all values other than density constant...

General form of fluxes:

$$\Gamma_{i+\frac{1}{2}} = \sigma(\frac{\lambda}{e^{\lambda dx} - 1} n_{i+1} + \frac{\lambda}{e^{-\lambda dx} - 1} n_i)$$

Note density dependence from adjacent nodes!

Equations (2)

COMPUTATIONAL

Electron Sources*	Ion Sources*

$$S_e = \alpha|\Gamma_e| - \beta n_e n_i - \nu_a n^2 n_e$$

Ionization | Recombination | 3 - Body

$$S_i = \alpha|\Gamma_e| - \beta n_e n_i$$

Ionization | Recombination

- Semi-implicit time-stepping method
  - Allows for larger time-steps
  - Lower computation time

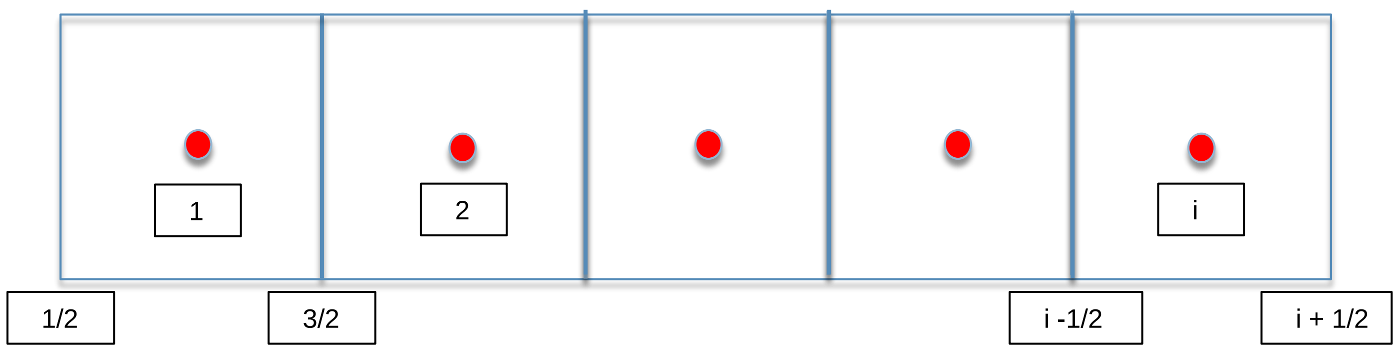
$$\frac{n_i^k - n_i^{k-1}}{\Delta t} + \frac{\Gamma_{i+\frac{1}{2}} - \Gamma_{i-\frac{1}{2}}}{\Delta x} = S \qquad \Gamma = \Gamma(n^k, \Phi^{k-1})$$

*Ignored negative ions

Mesh

COMPUTATIONAL

1-D Example:



SG assumes all variables other than density constant across a cell *i*

- calculated on the boundaries of the cells

Wall Boundary Conditions

COMPUTATIONAL

- Boundary conditions applied on flux nodes
  - Somewhat difficult to find ones that made sense physically and numerically
- Current BC:
  - Assuming small gradients of temperature & density
  - Up-wind scheme → assume fluxes always going into the wall
    - Unsure about this condition but presents the best results

$$n_1^k + \frac{\Delta t}{\Delta x}[(a\mu E n_e)_1 + (b\mu E n_e)_2)] = S + n_1^{k-1}$$

← Left Boundary

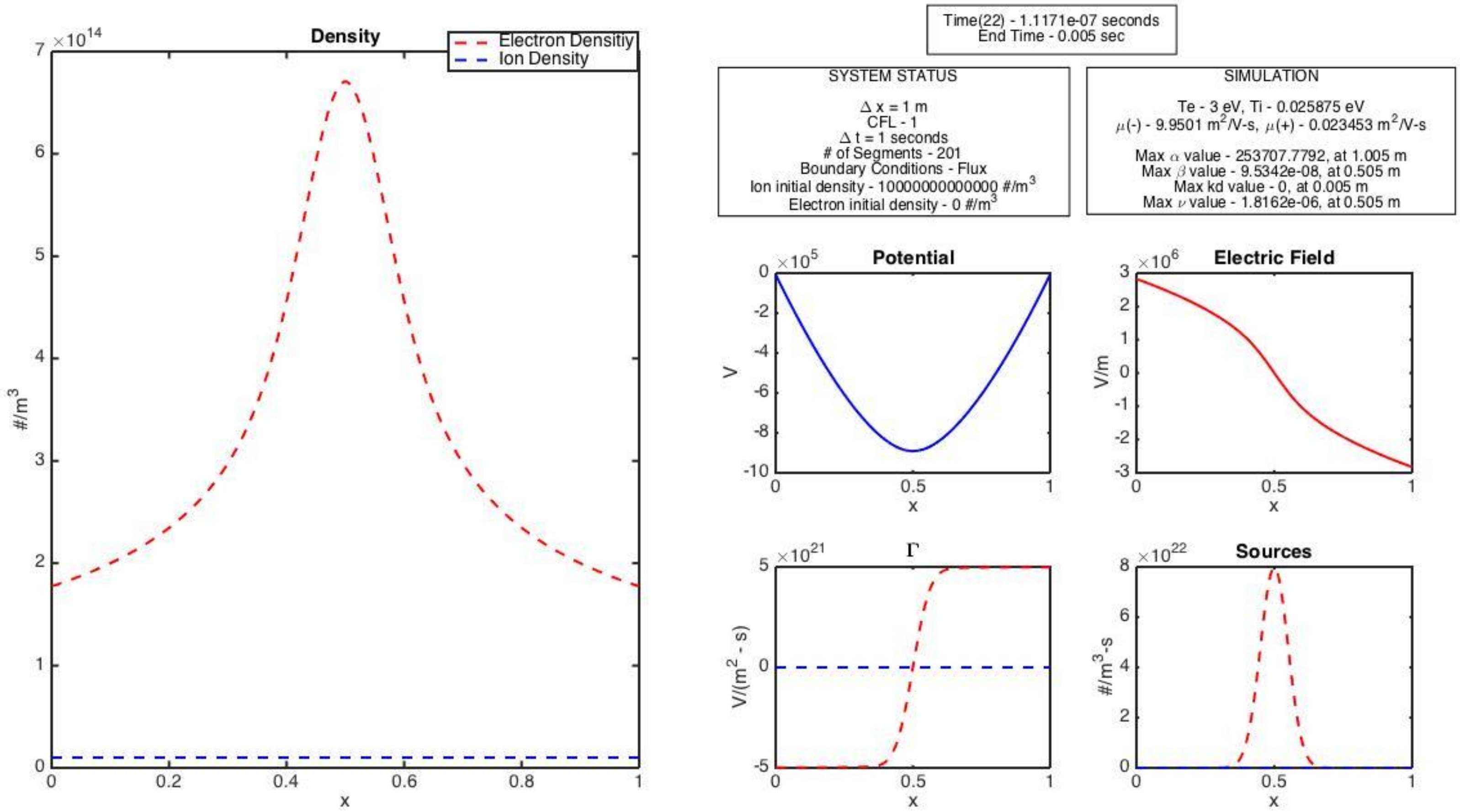
Right Boundary →

$$n_x^k + \frac{\Delta t}{\Delta x}[(a\mu E n_e)_x + (b\mu E n_e)_{x-1})] = S + n_x^{k-1}$$

a and b → coefficients to ensure upwind towards boundaries

Electrons – Gaussian Source

COMPUTATIONAL

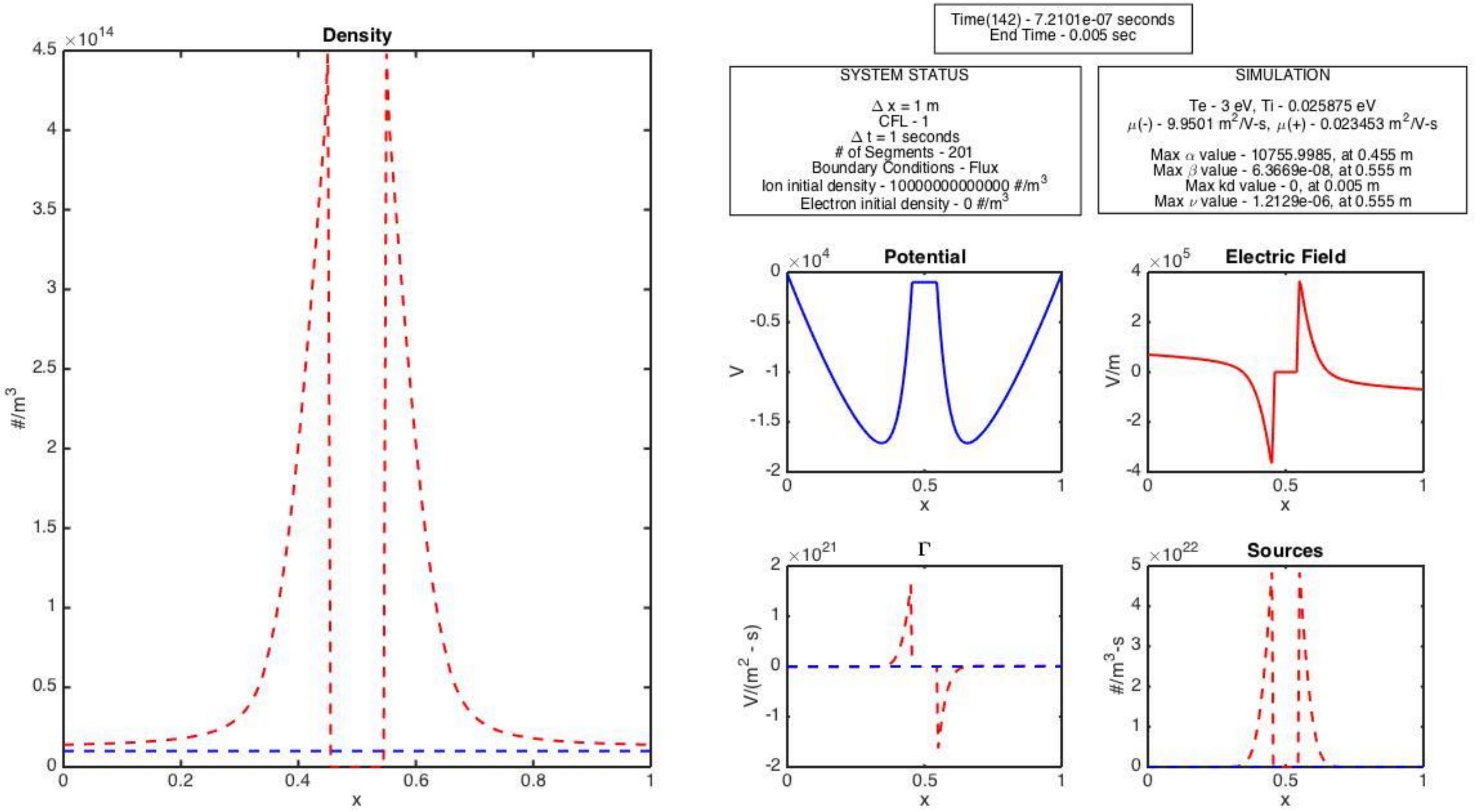


Extractor Plates

- Extractor plates required to accelerate electrons
- 1-D simulation
  - Imposed potential on a plate in the middle
  - Wall boundaries on plate edges
- In 2-D simulation
  - Used to extract electrons and accelerate to desired energy levels

Electrons – Gaussian Source + Emitter

COMPUTATIONAL



Future Work

Future Work

- Numerical Analysis
  - Implement sources/sinks into model
    - Ionization/recombination coefficients
  - Boundary conditions
  - Extend to 2-D
    - Extractors
    - Control electron energy levels
    - Model collisions with N_2O
- Experimental setup
  - Design electron source
  - Isolate excited states of nitrous oxide
- Main goal: Achieve self-sustained decomposition

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FUTURE WORK

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Questions?