IPT – Direct Power Extraction

NETL Office of Research and Development

2016 Crosscutting Technology Research Review Meeting

Rigel Woodside, Tom Ochs, David Huckaby, James Bennett, Hyoungkeun Kim, Eric Zeuthen, Jin Nakano, Anna Nakano, Clint Bedick, Duncan McGregor, Danylo Oryshchyn, John Lineberry

Presentation Focus & Outline

Direct Power Extraction (DPE): technology which directly converts thermal/kinetic power to useable electrical power.

DPE Example: magnetohydrodynamic (MHD) generator. This is our present focus, and in particular we focus on the unique challenges of this.

DPE Task Goal: Generate engineering data sets, simulation tools, and materials to further the prospect of using DPE

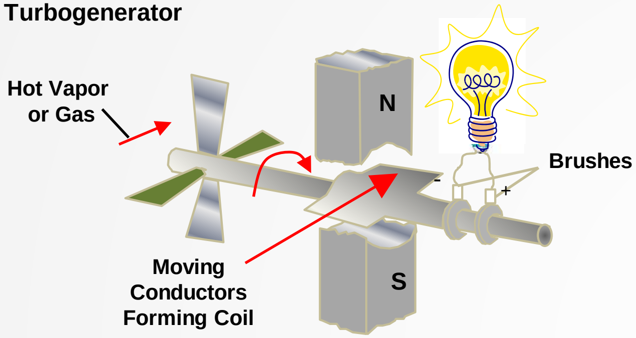
- **Introduction**
- **Electrical Conductivity for Open Cycle Application**
- **Computational MHD for Performance Assessment**
- **Operation & Simulation of HVOF Combustion Process**
- **Electrode Exposure Testing**
- **Conclusion**

MHD Power Generator

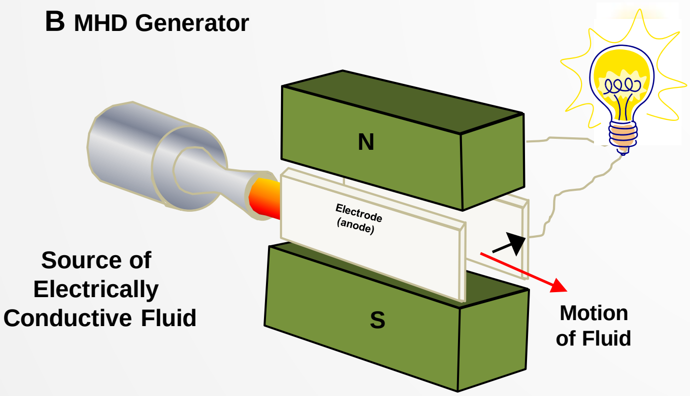
A. **Turbo-generator Energy Conversion -> chemical (fuel) to thermal/kinetic to mechanical to electric**

B. **MHD Generator Energy Conversion -> chemical (fuel) to thermal/kinetic to electric**

A Turbogenerator



B MHD Generator



(more) Direct Power Extraction

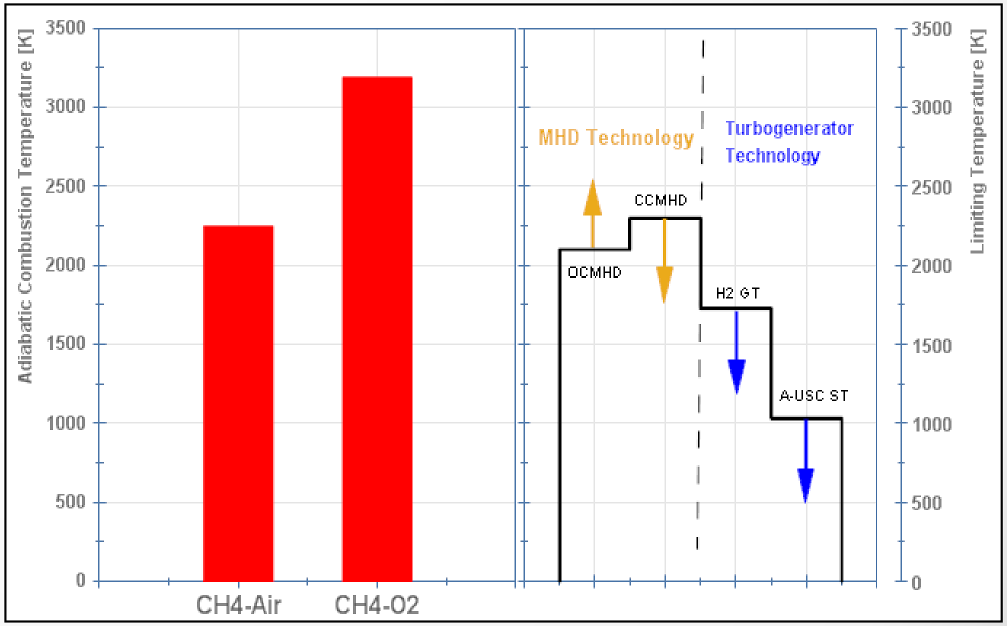
$$P \propto \sigma u^2 B^2$$

where B is applied magnetic field
σ is gas-plasma conductivity
u is gas-plasma velocity

- **“Step Increase” power generation efficiency**
  - By using much higher cycle temperatures

Carnot Limit $n_{th} \leq 1 - \frac{T_C}{T_H}$

- **Advantageous as topping cycles**
  - Non-disruptive to existing technologies
- **Improved CO_2 capture performance**
  - Synergistic with oxy-fuel approach
- **Flexible systems**
  - Coal + natural gas + bio-fuels
- **Compact systems**
  - Small footprint & potentially portable



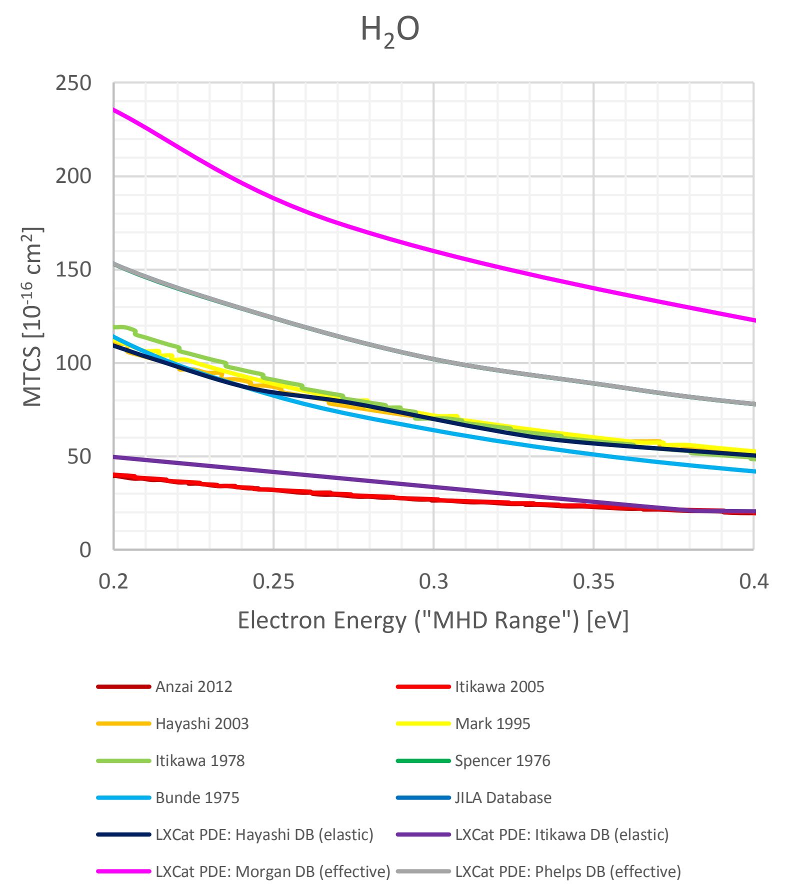
Key trends: Improving magnets & O_2 production

Electrical Conductivity of Seeded Oxy-fuel

- **Open-Cycle MHD scenario**
  - Traditionally uses alkali "seed" for electrons
    - K ~4.3 eV to ionize
    - K_2CO_3 stable and dissolves in water
  - Oxy-fuel combustion
    - (e.g. $CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$ at $\phi = 1$)
  - Determining Electrical Conductivity
    - Utilize Cantera for chemistry, ionization
    - $T_e = T_g$; Electrons all at mean speed
    - Neglects ion-electron collisions
    - Scalar (no magnet effect)

$$\sigma = \frac{n_e e^2}{m_e c_e \sum_k n_k Q_k} \qquad c_e = \langle v \rangle = \sqrt{\frac{8k_bT}{\pi m_e}}$$

n_e = electron number density [#/m^3]
e = electron charge = 1.60 x 10^{-19} [C]
m_e = electron mass = 9.11 x 10^{-31} [kg]
c_e = random thermal electron velocity [m/s] (estimated by the Maxwell-Boltzmann mean speed, $\langle v \rangle$)
n_k = neutral species number density [#/m^3]
Q_k = neutral species momentum transfer collisional cross section [m^2]
k_b = Boltzmann constant = 1.38 x 10^{-23} [J/K]
T = electron temperature [K]

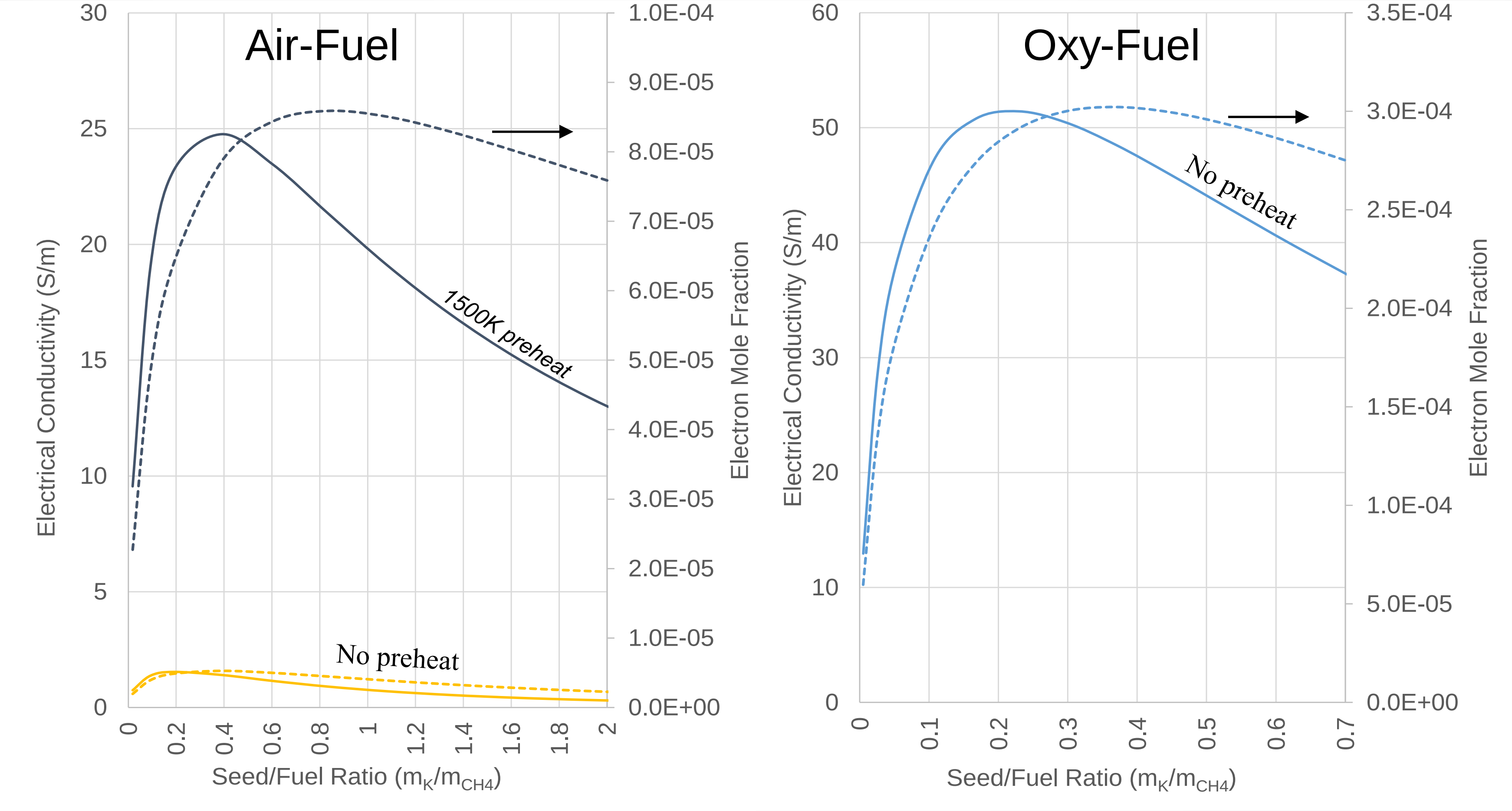


→ use $Q_k = f(T_e)$;

- Uncertainty from MTCS data significant
- H2O most important species for Q_k
- Paper forthcoming on recommend MTCS
  - Meta-analysis of ~100 sources

Electrical Conductivity Calculated Results 1/2

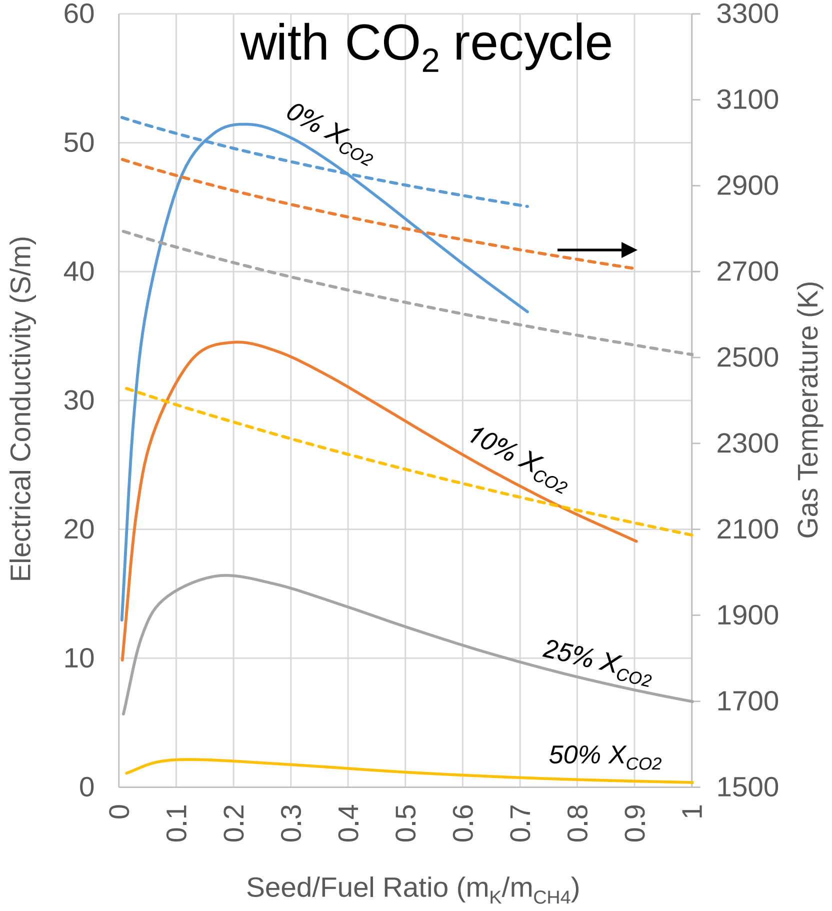
Results are for 1 atm. pressure combustion, 400K Inputs, 50/50 water/K_2CO_3 seed (pre-vaporized)
-note conductivity results will also be dependent on pressure-

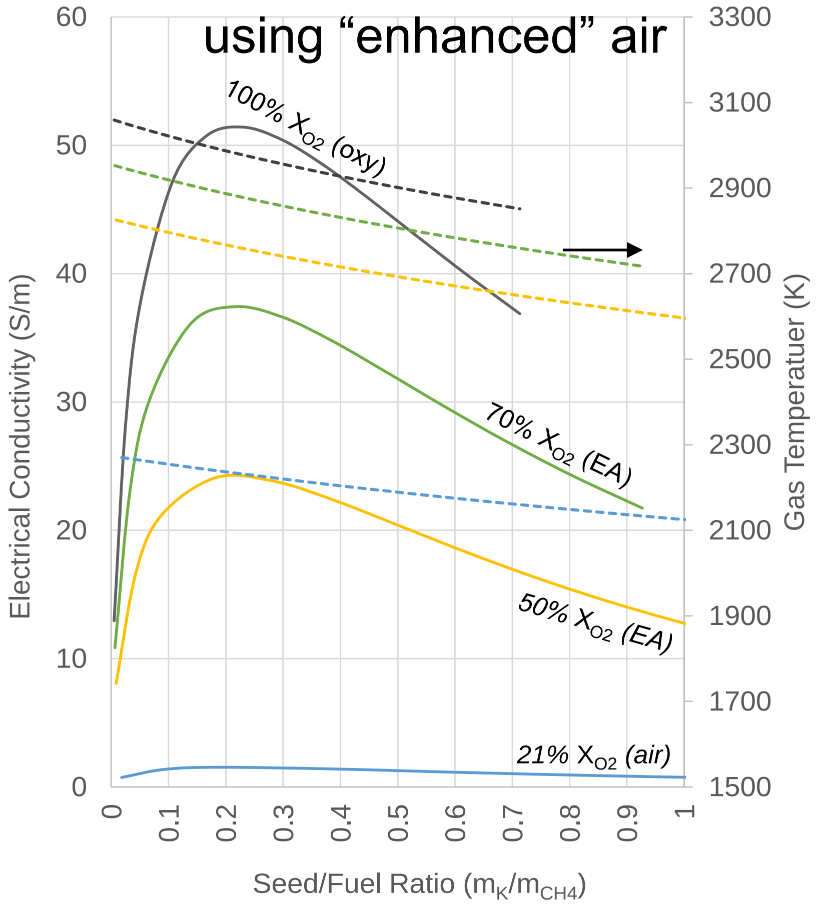


- Significant quantity of seeded needed in the system
- Peak electrons and peak conductivity not at same seeding level
- Pure oxy-fuel combustion 2x ~ conductivity of aggressive air pre-heat
- Less seed needed to reach conductivity peak for oxy-fuel vs air

Electrical Conductivity Calculated Results 2/2

Results are for 1 atm. pressure combustion, 400K Inputs, 50/50 water/K_2CO_3 seed (pre-vaporized)
-note conductivity results will also be dependent on pressure-



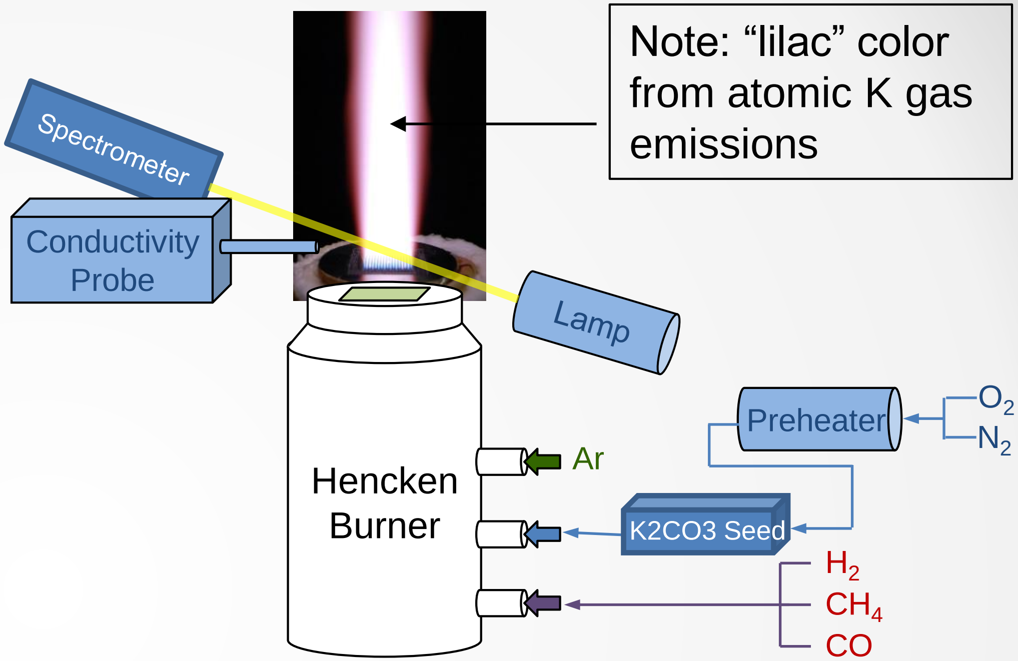


- Significant impact on conductivity from dilution -> very sensitive to temperature
- Dilution does not significantly impact optimal seeding level (no pre-heat added)
- Nitrogen dilution slightly more favorable then CO_2 dilution in terms of conductivity
  - Also true at comparable temperatures

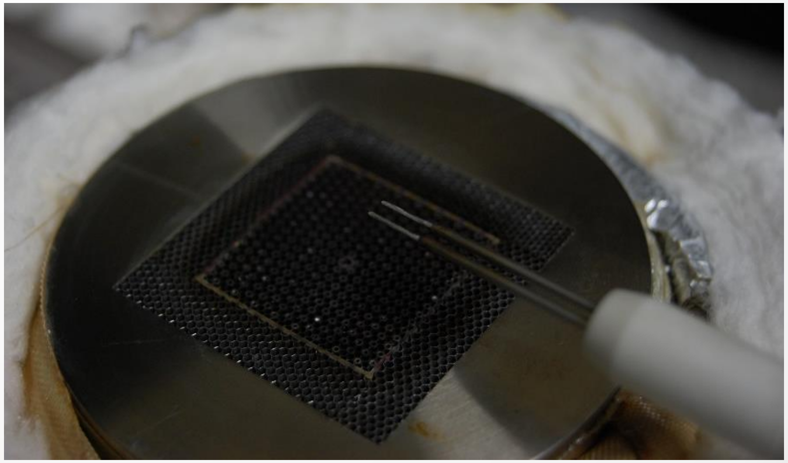
Conductivity Validation Experiment

Lab scale oxy-methane burner with seeding

- **Custom Hencken burner for oxy-fuel operation**
- **Langmuir double probe w/ custom platinum/tungsten tips**
  - Current measured at discrete voltage steps
    - $\sigma \propto I/V$
  - Rapid insertion/removal (30-50ms)
- **Seeding system undergoing improvement**
  - Capable of up to 5% (by wt.) K introduction
  - 50/50 K_2CO_3/H_2O solution
  - Syringe pump for solution delivery
  - Ultrasonic nozzle to atomize in oxidant stream
  - Heat tracing to evaporate water prior to burner
- **Utilizing CCD Spectrometer**
  - For absorption spectroscopy of atomic K (concentration, flame temp)



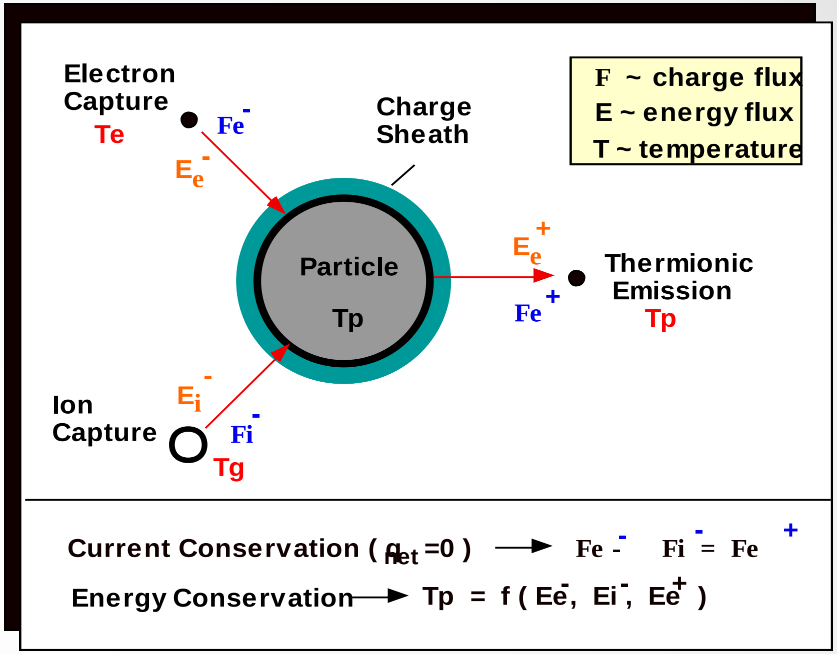
Note: “lilac” color from atomic K gas emissions



Alternative Approach: Dusty Plasma 1/2

Instead of an alkali seed

- **Plasma Conductivity via condensing nano-droplets, i.e., “a dusty plasma”**
  - Some oxide compounds exhibit a lower thermionic emission energy than ionization energy and can produce free electrons at lower temperature
  - Process is a quasi-equilibrium state at given T
  - Effective particle surface emission implies:
    - Very small ideal: ~ submicron size needed
    - Technical challenge to produce and control
  - Lower temperature MHD cycle is possible and concept has potential compatibility with direct fired gas turbine
    - Due to small particle size no blade erosion
    - Enabling concept for triple cycle..MHD + NGCC, i.e., potentially promising carbon capture route for Natural Gas



Current Conservation ($q_{net} = 0$) $\longrightarrow$ $Fe^- - Fi^- = Fe^+$

Energy Conservation $\longrightarrow$ $Tp = f(Ee^-, Ei^-, Ee^+)$

- ✓ Energy and Current conservation at given T
- ✓ Free electron number density, Ne, can be expressed as,

$$N_e = 2\,\frac{(2\,\Pi\, m\, k\, T)^{\frac{3}{2}}}{h^3}\,\exp\, -\left(\frac{\Phi_{wf}}{kT} + \frac{e^2 z}{r_s\, kT}\right)$$

Φwf ~ work function

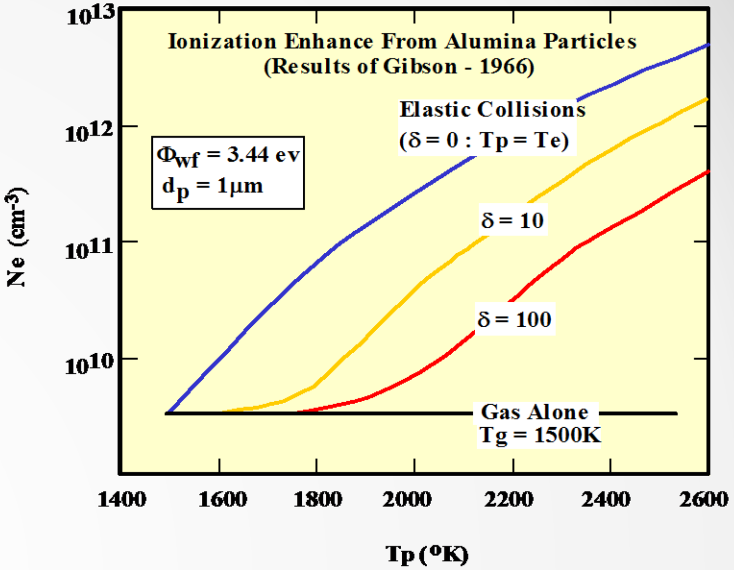
rs ~ particle radius

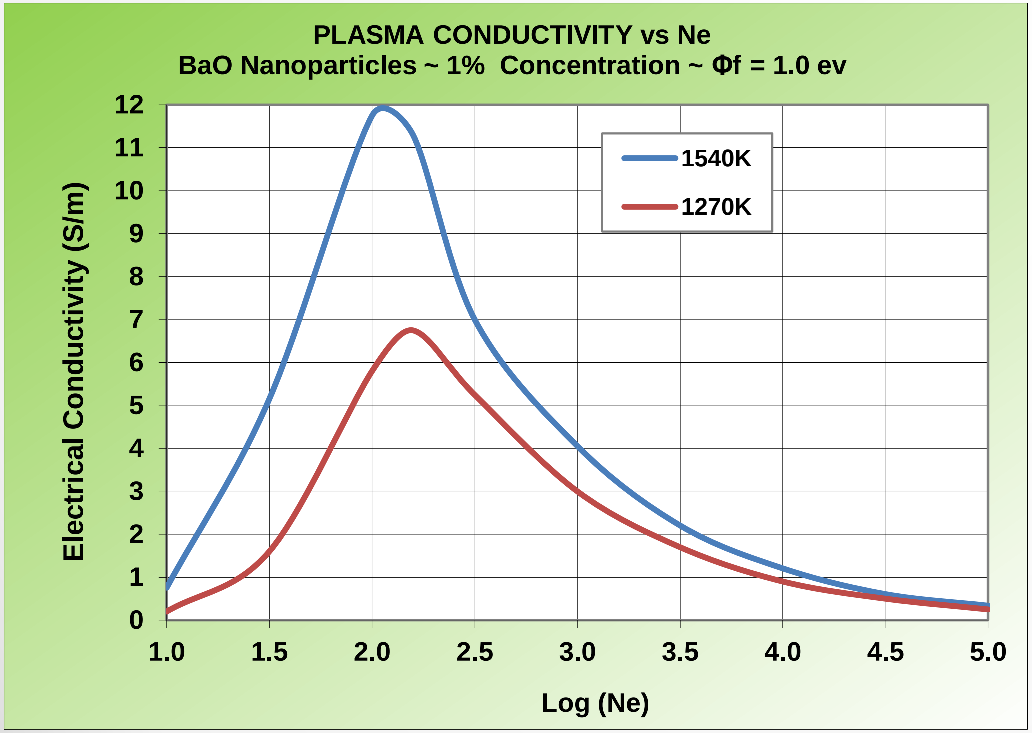
Above sketch from by Lineberry, 1993

Alternative Approach: Dusty Plasma 2/2

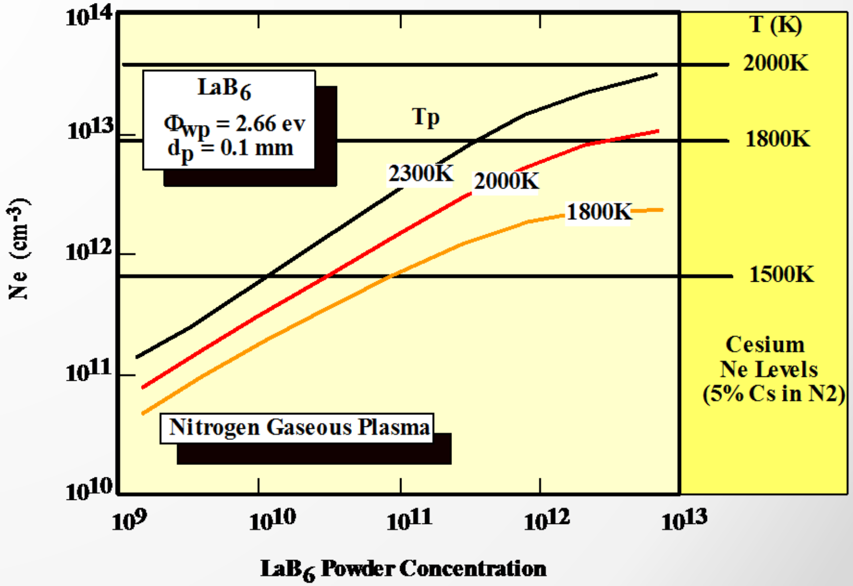
Instead of an alkali seed

- **Ceramic oxides are promising candidates**
    - low work function
    - Compatible vapor P-T properties
    - High dissociation energies





Ionization Enhance From Lanthanum Hexaboride Particles
(Results of Honma - 1968)

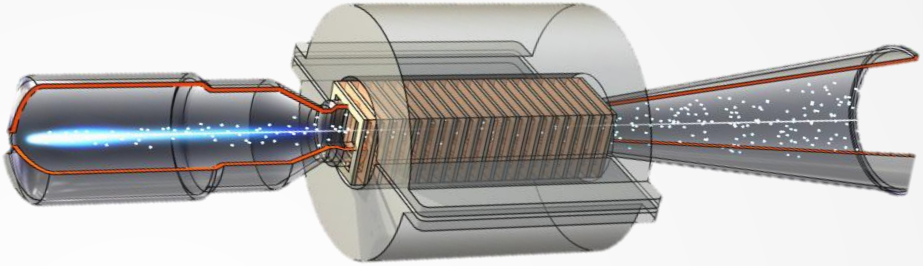


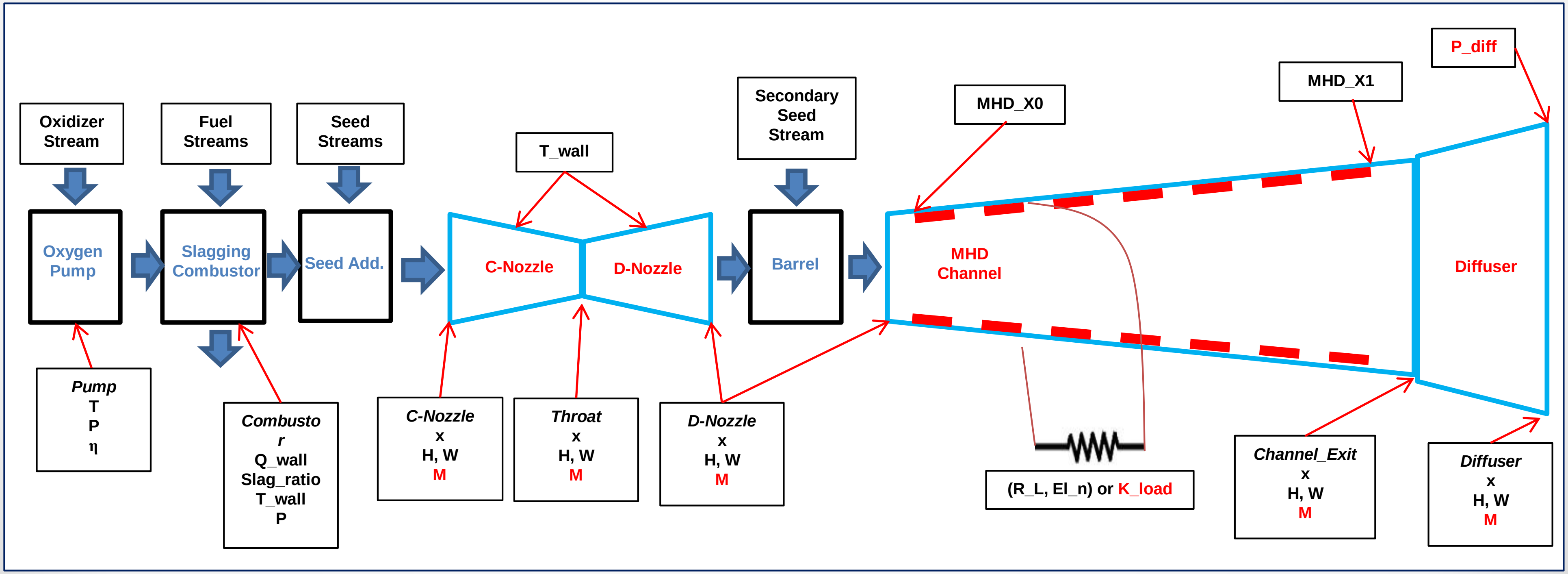
Simulation: NETL’s 1D MHD code

- **Significant inputs**
  - Mass flow & Inlet species mixture
  - Target channel Mach # or Channel geometry
  - Magnetic Field Profile
  - Diffuser outlet pressure
  - External channel load (K or resistance)
- **Significant outputs**
  - Power Generation & Heat Losses
  - Channel Dimensions & Flow profile
- **Typical channel design constraints**
  - Critical current density
  - Critical hall voltage

Developed to to Specify a MHD “Power train”

Combustor | Channel | Diffuser





Oxidizer Stream

Fuel Streams

Seed Streams

T_wall

Secondary Seed Stream

MHD_X0

MHD_X1

P_diff

Oxygen Pump

Slagging Combustor

Seed Add.

C-Nozzle

D-Nozzle

Barrel

MHD Channel

Diffuser

Pump
T
P
η

Combustor
Q_wall
Slag_ratio
T_wall
P

C-Nozzle
x
H, W
M

Throat
x
H, W
M

D-Nozzle
x
H, W
M

(R_L, El_n) or K_load

Channel_Exit
x
H, W
M

Diffuser
x
H, W
M

Code is run iteratively to optimize system. Utilized in NETL’s DPE techno-economic studies

Simulation: 1D MHD code methodology

Numerical methods: Governing equations solved as an initial value problem given the inlet conditions. The equations are a DAE (differential algebraic equation) system.

$$\text{Mass}: \frac{d}{dx}(\rho u A) = 0$$

$$\text{Species}: \rho u \frac{dY_k}{dx} = R_k W_k$$

$$\text{Momentum}: \rho u \frac{du}{dx} + \frac{dP}{dx} = F_{EM} - F_{friction}$$

$$\text{Energy}: \rho u \left(u \frac{du}{dx} + \frac{dh}{dx} \right) = P_{EM} - Q_{wall} - Q_{rad}$$

$$\text{Boundary}: \frac{d\theta}{dx} + \frac{\theta}{u}\frac{du}{dx}\left(2 + \frac{\delta^*}{\theta} - M^2\right) = \frac{1}{2} C_f$$

$$\text{Lorentz}: F_{EM} = J_y B_z$$

$$\text{Power}: P_{EM} = J_y E_y + J_x E_x$$

Programming language:

Python, Numerical libraries use C, C++ and Fortran

Key libraries:

Cantera – thermodynamics, transport and reactions
Assimulo – interface for SUNDIALS
SUNDIALS – DAE integration package from Sandia

- 5 main equations (**mass**, **momentum**, **energy**, **chemical reaction**, **boundary layer**) for the flow state.
- 2 equations (generalized Ohm's law) for the EM field.
- Additional equations for Channel to account for:
  - Electrode Configuration
  - External Load

$$J_x = \frac{\sigma}{1+(\omega\tau)^2}\left[E_x - \omega\tau E_y + \omega\tau u B_z\right]$$

$$J_y = \frac{\sigma}{1+(\omega\tau)^2}\left[\omega\tau E_x + E_y - u B_z\right]$$

$$E_x = \frac{1}{\sigma}(J_x + \omega\tau J_y)$$

$$E_y = \frac{1}{\sigma}(-\omega\tau J_x + J_y + \sigma u B)$$

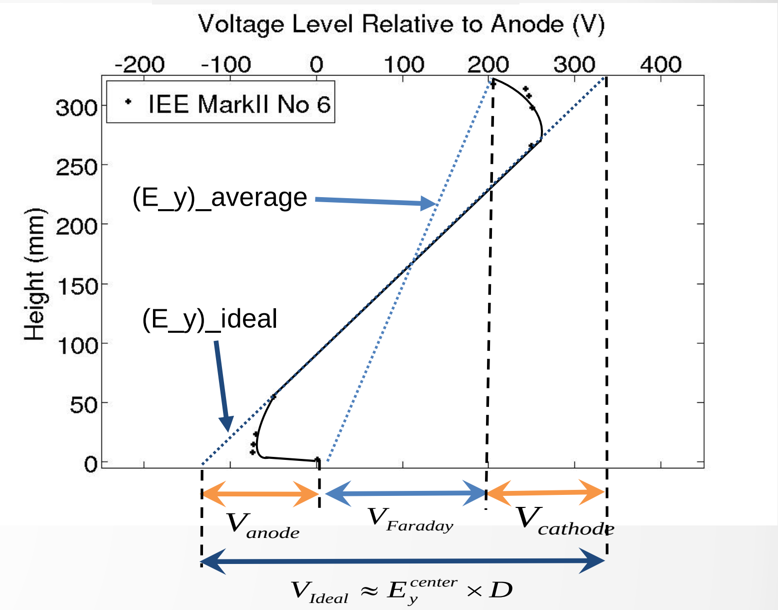
The code calculates the variable power outputs along channel length.

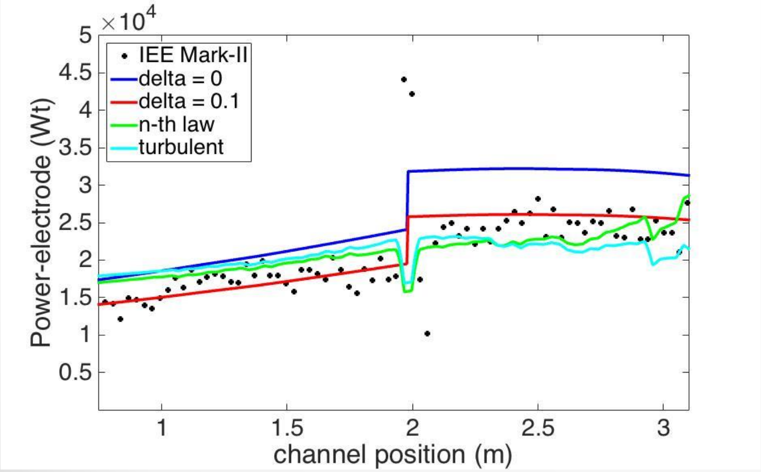
1D “+” code enhancement

To approximate effects of parameters inadequately described in a 1D model

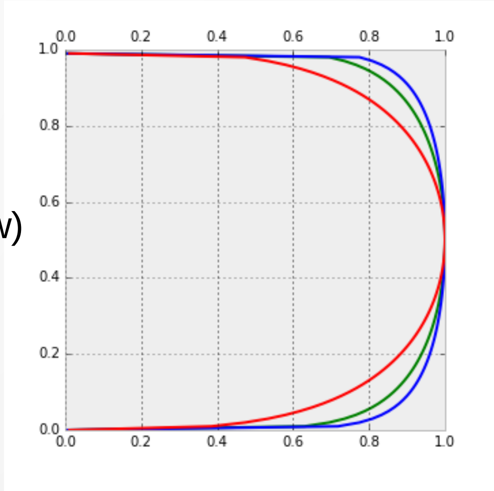
- **Boundary layer voltage drop:**
  - Correct current and E-field to account for the low near wall conductivity due to the lower wall temperature the conductivity and other non-idealities (electrode resistances …)
  - For Ideal Segmented Faraday Channel: $J_y = (1-K)\sigma u B(1-\Delta)$
  - $V_{drop} = \Delta u B D$
  - external “loading factor (K)” or “resistance (Ω)” provided
- **Constant Voltage drop ratio (robust & fast) :**
  - Δ - unique to a system calculated using ratio (electrode spacing to boundary layer thickness) typical value ~ 0.1
- **Profile Methods**
  - Δ = Δ(x)
  - Assume boundary layer resistance dominates
  - Integrate Ohm’s law given the conductivity profile
  - Conductivity profile derived from a temperature profile
  - Temperature profile derived from 1D values (T, u, p), normalized velocity and total enthalpy profiles
    - “n^th-power law” & “turbulent” models have been implemented
  - Can also be used estimate Δ for constant voltage drop model

Lineberry 1988 AIAA





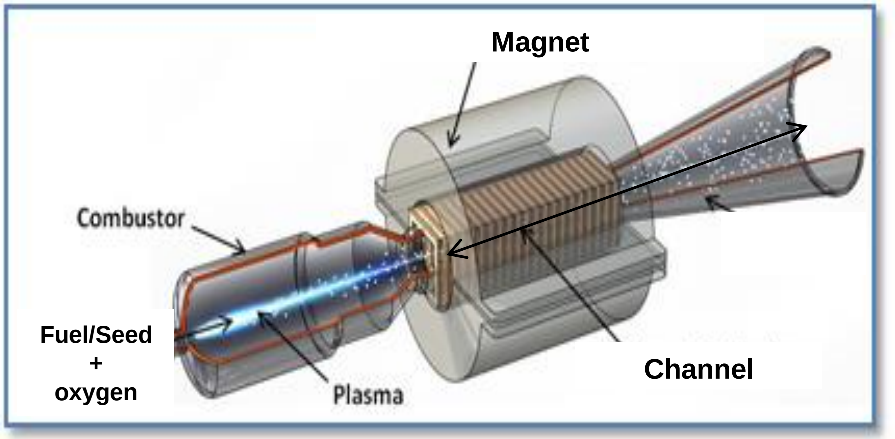
Red- conductivity
Blue – temperature (T-T_w)/(T_c-T_w)
Green – velocity (u/u_c)
Across channel cross section



NETL MHD Lab operations

- **NETL MHD lab focuses on simulation validation and channel material exposure testing**
- **2014: Design**
- **2015: Construction**
- **2016: Phase 1 MHD "component testing" underway**
  - ~2T Electromagnet
    - Set-up and model validation complete
  - ~200 kWt High Velocity Oxy-Fuel (HVOF) Gun
    - With seed injection
- **2016: Photoionization concept testing to begin**
- **2016: Basic channel coupon materials testing to begin**
- **2017: Introduce MHD channel section**
  - Initially "back powered" (power supplied to channel, no magnet)
  - FEM of thermal-structural for channel built
  - FEM of 3D current profiling and diagnostic for current density scoped
- **2018: MHD channel section testing capable of producing power**
  - Infrastructure ready to scale up to ~ 1MWt
    - Increased size needed to overcome boundary layer resistances
    - Note this is not a MHD power demo

"remote" MHD testing inside a 20' x 12' booth

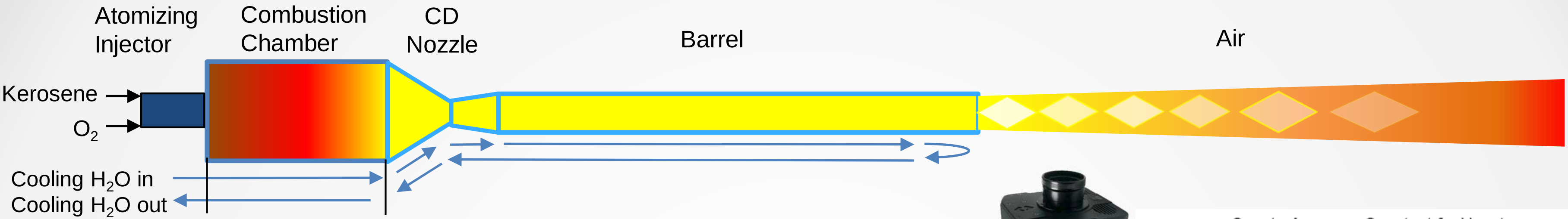


Goal is bench scale MHD Power train testing

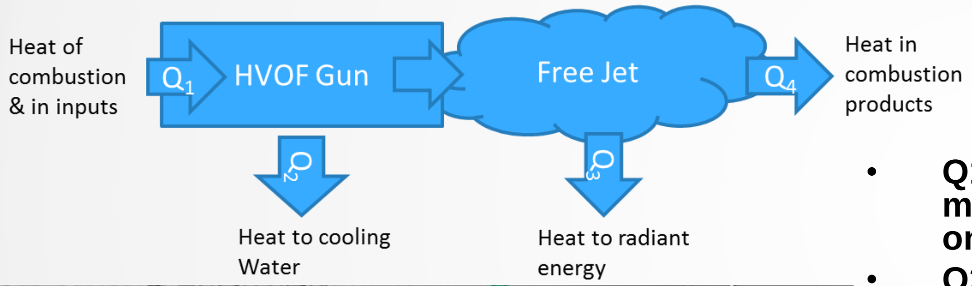
HVOF Heat Balance: Initial Sim. Val. Target

In order to establish important heat transfer parameters

Nominal firing rate: 177 kWt



Heat Balance



Heat of combustion & in inputs

Q_1

HVOF Gun

Free Jet

Q_4

Heat in combustion products

Q_2

Heat to cooling Water

Q_3

Heat to radiant energy

IR camera

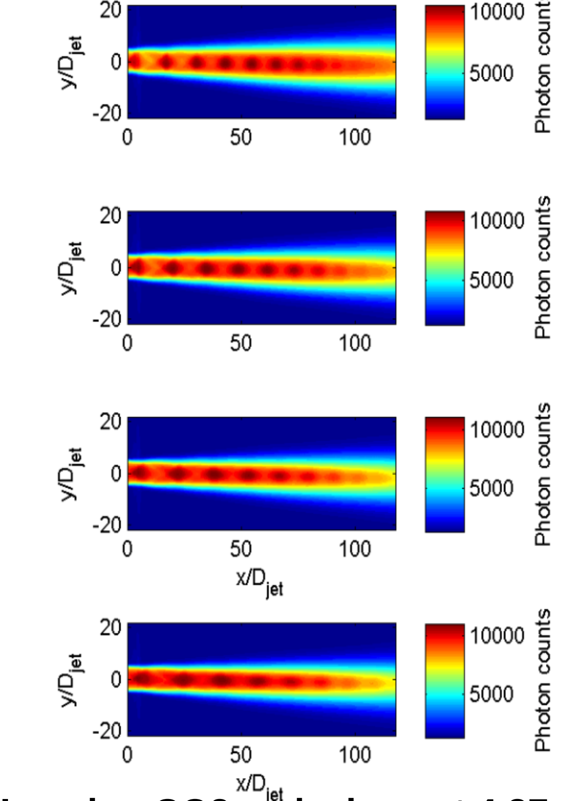
- **Q1: From Inputs: T, P, mdot + off-line HHV test on fuel**
- **Q2: From cooling water: mdot*Cp*dT; dT = T_{out}-T_{in}**
- **Q3: Use a Total Radiometer**
- **Q4: From the balance**

Preliminary data Suggests 20-25% Heat Loss to Walls (Q2)

Shock diamonds can be seen at HVOF exit

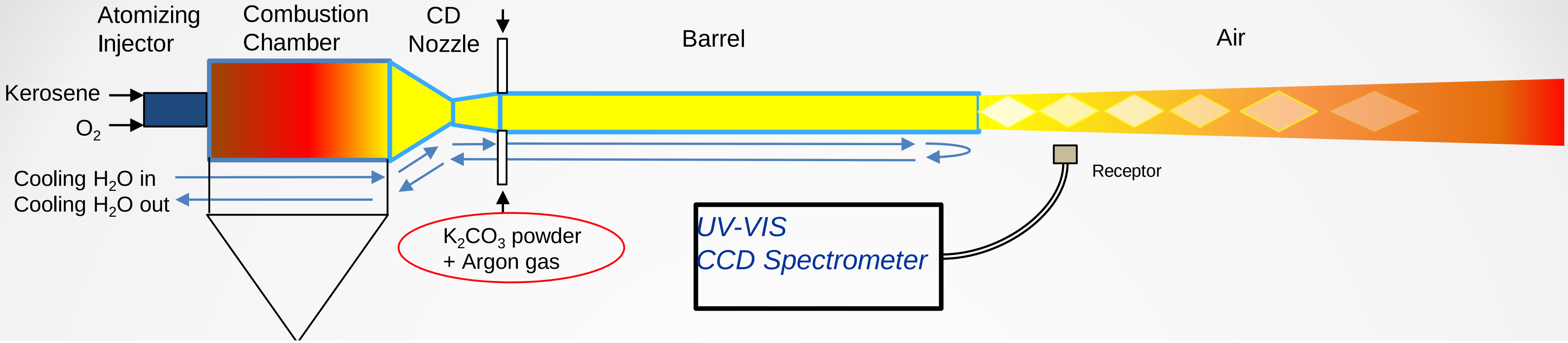
Counts Average. Constant fuel input.

Fuel- 4.2 GPH. Oxygen- 950, 1100, 1250 & 1400 SCFH.



Imaging CO2 emissions at 4.37 um

HVOF operation with K_2CO_3 injection



Atomizing Injector

Combustion Chamber

CD Nozzle

Barrel

Air

Kerosene

O_2

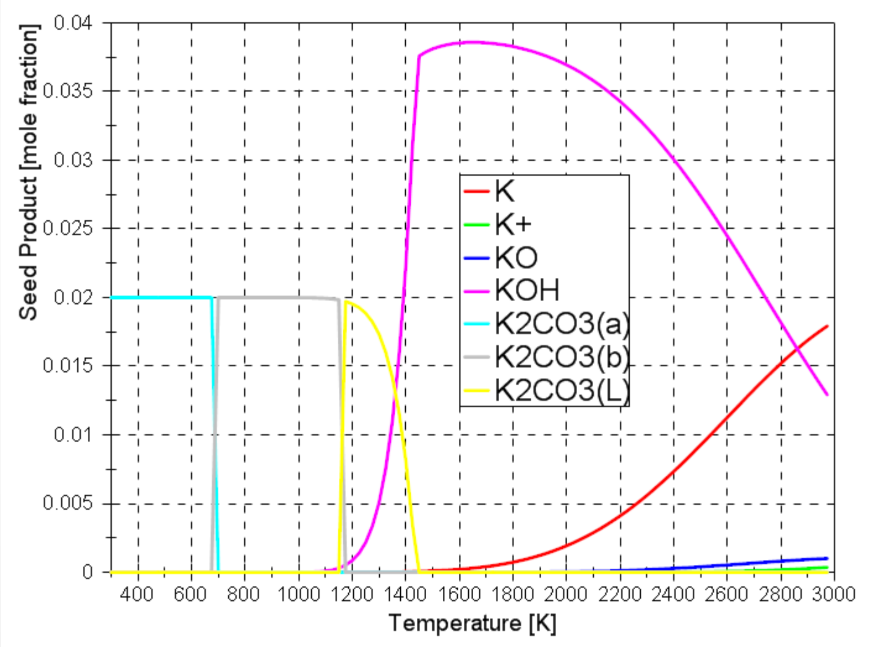
Cooling H_2O in

Cooling H_2O out

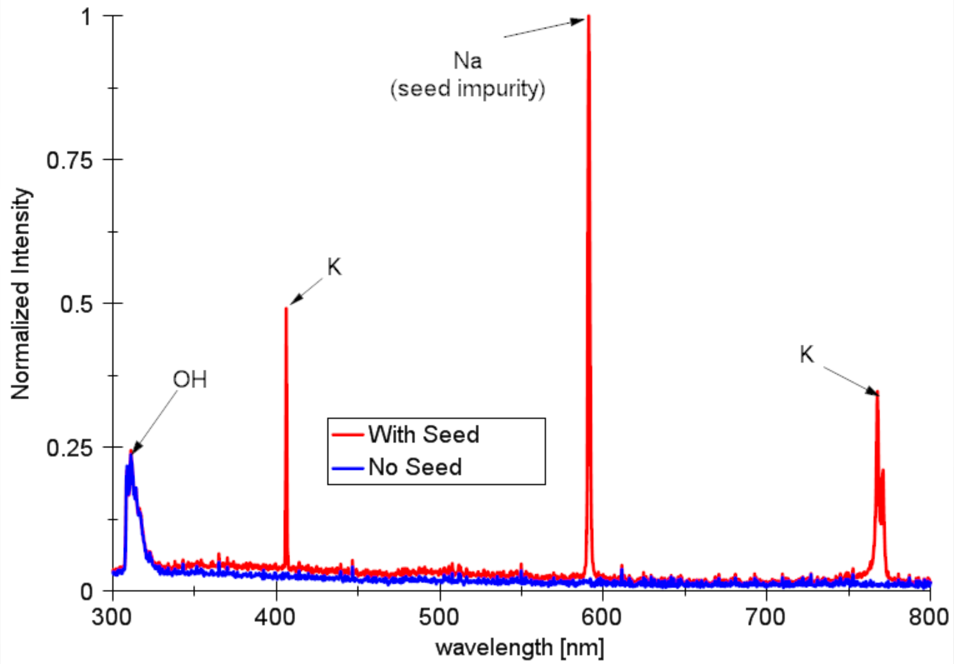
K_2CO_3 powder + Argon gas

UV-VIS CCD Spectrometer

Receptor



Equilibrium Phase diagram for oxy-fuel + K_2CO_3 seed



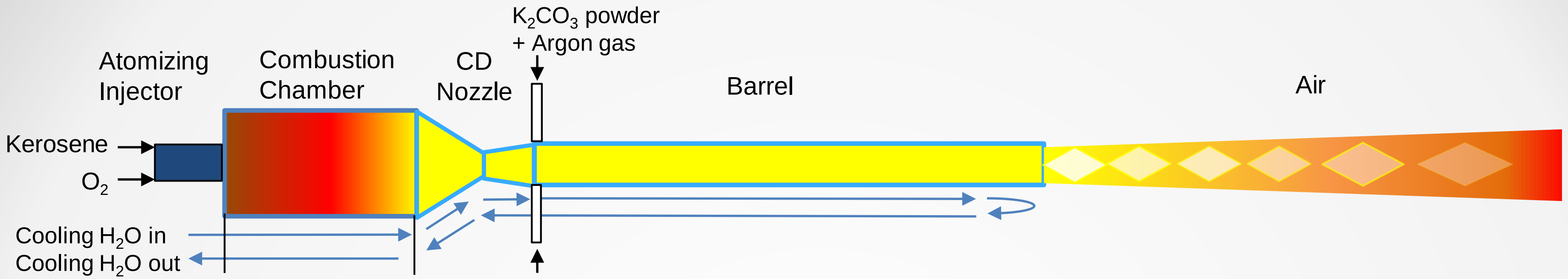
K_2CO_3 is vaporizing to K in experiment

-Planning in implementing Spectroscopic method

for K species density & temperature

Project is working toward experimentally obtaining mass balance of seed species.

HVOF Simulations



K_2CO_3 powder + Argon gas

Atomizing Injector

Combustion Chamber

CD Nozzle

Barrel

Air

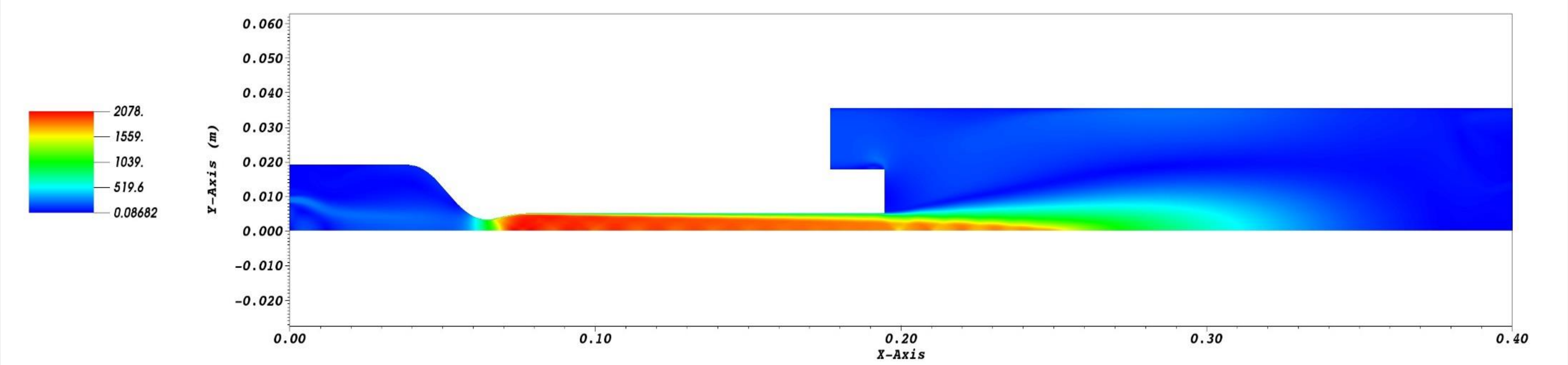
Kerosene

O_2

Cooling H_2O in

Cooling H_2O out

Axisymmetric system, simulated with “1/4” slice. Irregular mesh at diverging nozzle

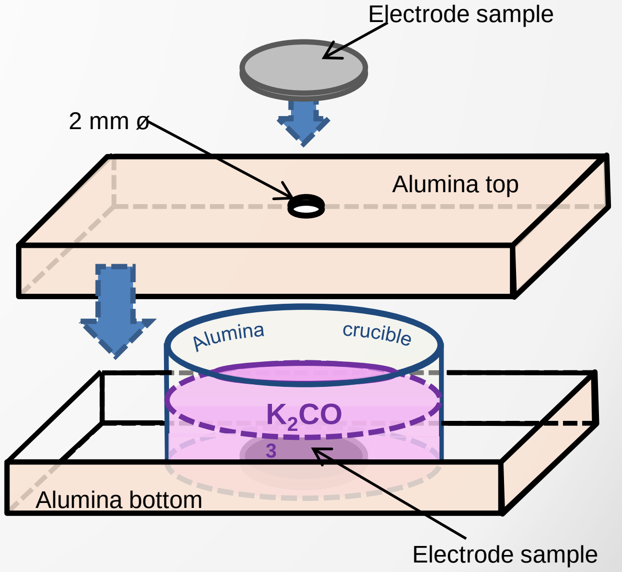


- Shock structure apparent in simulations: Exact geometry optimized using MOC
  - Free jet appearance qualitatively similar to IR measurements
- Initial validation Target will be heat balances (with no seeding)
  - Wall heat loss calculation using OpenFOAM utility “wallHeatFlux”
  - Utilize Free Jet radiation solver in OpenFOAM
- Seed concentration profile and conductivity will be examined in simulation

MHD Electrode Testing

- **General Electrode Requirements**
  - Good electrical conductivity
  - Adequate thermal conductivity
  - Resistance to electrochemical corrosion (seed/slag)
  - Resistance to erosion by high velocity particle laden flow (seed/slag)
  - Resistance to thermal shock
  - Compatibility with other materials in system
  - Resistance to/minimization of arc attack/erosion

- **Expose samples to K_2CO_3**
  - Based on ASTM test C987 -10
  - 48 hrs. at 1500°C in air (semi-closed w. lid)
  - Atmosphere is air
    - Planning for Additional testing in CO_2 environment
  - Both liquid and vapor exposure tests



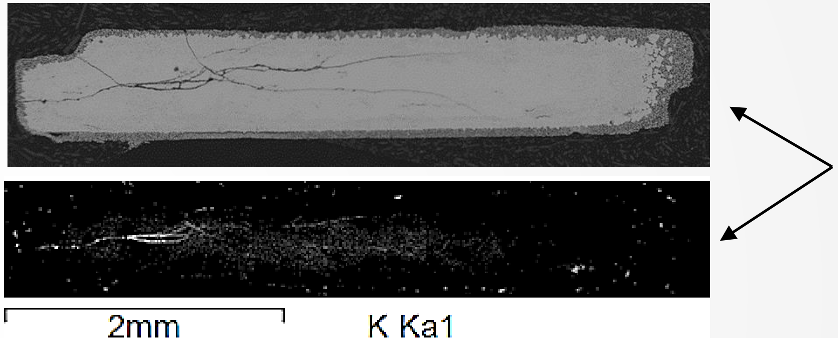
- **Ex-Situ exposure characterization**
  - Mass Change measurements
  - SEM imaging of microstructure
  - SEM-EDS for surface chemistry profiling
  - XRF for bulk chem. and XRD for phase identification
  - Optical Microscopy for surface analysis

Electrode Exposure to K_2CO_3

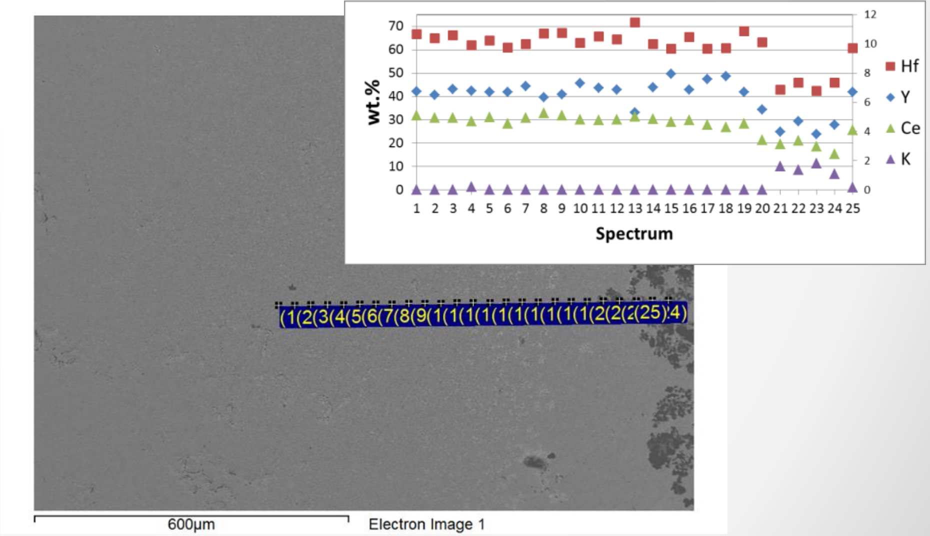
- **Four “reference” MHD electrodes tested**
  - Materials considered or tested in MHD channel in the past
  - Fabricated with pressure less sintering

Materials tested	Weight change (%)*
Samples exposed to the K_2CO_3 Liquid	
1. $88\%ZrO_2$-$12\%Y_2O_3$	-10.9
2. $89\%ZrO_2$-$10\%Sc_2O_3$-$1\%Y_2O_3$	-20.2
3. $83\%HfO_2$-$17\%In_2O_3$	-100.0
4. $82\%HfO_2$-$10\%CeO_2$-$8\%Y_2O_3$	-7.6
Samples exposed to the K_2CO_3 Vapor	
1. $88\%ZrO_2$-$12\%Y_2O_3$	-0.8
2. $89\%ZrO_2$-$10\%Sc_2O_3$-$1\%Y_2O_3$	0.0
3. $83\%HfO_2$-$17\%In_2O_3$	-18.5
4. $82\%HfO_2$-$10\%CeO_2$-$8\%Y_2O_3$	0.0

$82\%HfO_2$-$10\%CeO_2$-$8\%Y_2O_3$ – exposed to K_2CO_3 liquid



Sample Cracking Visible w/ K present



- K liquid exposure increased degradation compared to vapor exposure
- Opening of grain boundaries and pores upon gas exposure.
- Polished surfaces seemingly were less affected by liquid exposure

Future work: Exposure Prospective Electrodes to the HVOF In the MHD lab

Conclusions

- **Oxy-fuel significantly boosts conductivity of alkali seeded OCMHD systems**
  - Slightly less seed also needed
  - Validation testing for conductivity of seeded oxy-fuel underway
- **Thermal ionization of Alkali seed may not be only OCMHD option**
  - Photoionization and dusty plasma being investigated
- **A 1D code has been implemented for detailed specification of an MHD power train**
  - Multi-dimensional effects can still be considered
- **Heat losses are significant for small scale OCMHD systems**
- **Reactivity to seed compounds can be severe for electrodes**

Questions?