Pulse Detonation Engine for Power Extraction from Oxy-Combustion of Coal-Based Fuels

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Funding from NETL (FE0025822), Oregon BEST

PROPULSION LABORATORY

NRG

CIRE Lab

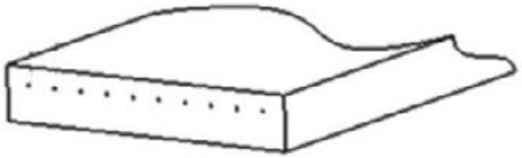
Acknowledgements

Students: Matthew Zaiger, Derek Bean, Shahank Karra, Rachel Nelke, Peter Beck, Zach Powell, Austin Rose, Matthew Hoeper (Oregon State University), Daiki Ichinokiyama (University of Tsukuba)

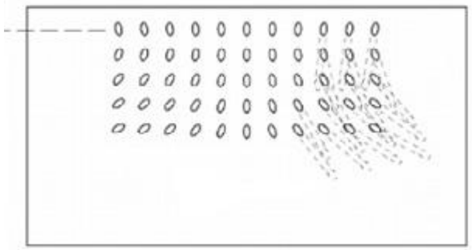
Collaborators: Drs. Fred Schauer, John Hoke and team at Air Force Research Laboratory.

Motivation

- Improvements in thermodynamic efficiency of power plants needed
- Pressure gain combustion using detonations can significantly improve efficiency



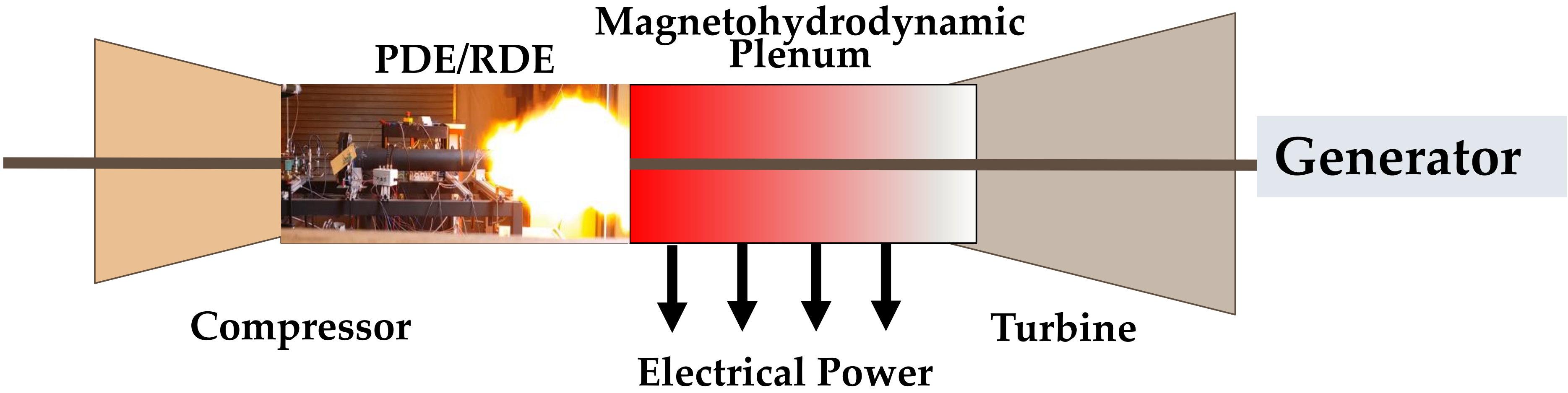
Normal Holes



Shaped Array

Richardson, Blunck et al., Combustion and Flame 2016

Motivation



PDE/RDE

Magnetohydrodynamic Plenum

Generator

Compressor

Electrical Power

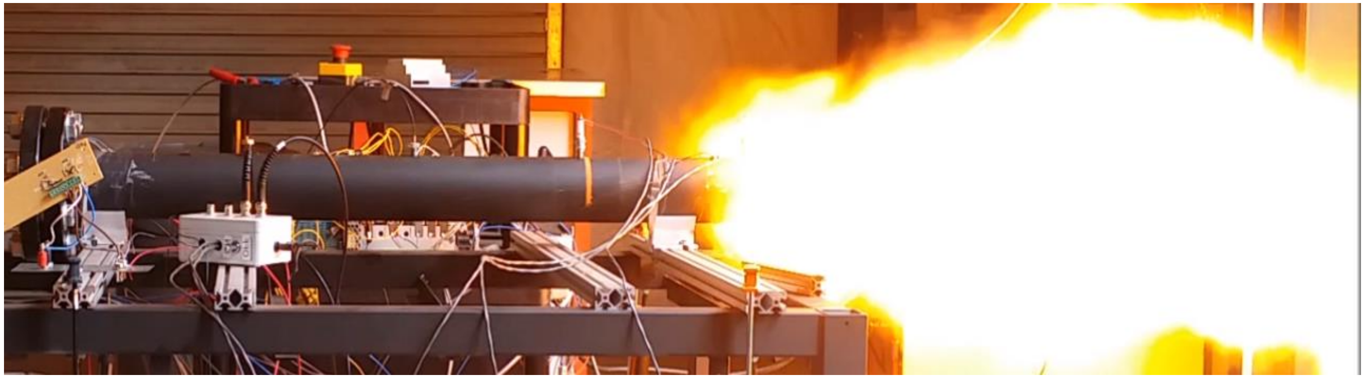
Turbine

Advantages of detonation-fed MHD: $P \propto \sigma \times V^2 \times B^2$

- High velocities (Ma > 2)
- High temperatures (T > 3000 K) increase electrical conductivity

Key Findings

1) Particle seeder developed for unsteady detonations
2) Data collected for CH_4-O_2 detonations
3) Electrical conductivity measurements being collected, preliminary results indicate seeding needed
4) Ionization chemistry of seed particles reduces detonation speed
5) Detonation solver developed for oxygen-fuel combustion
6) Residual combustion products suppress detonations



Technical Objectives

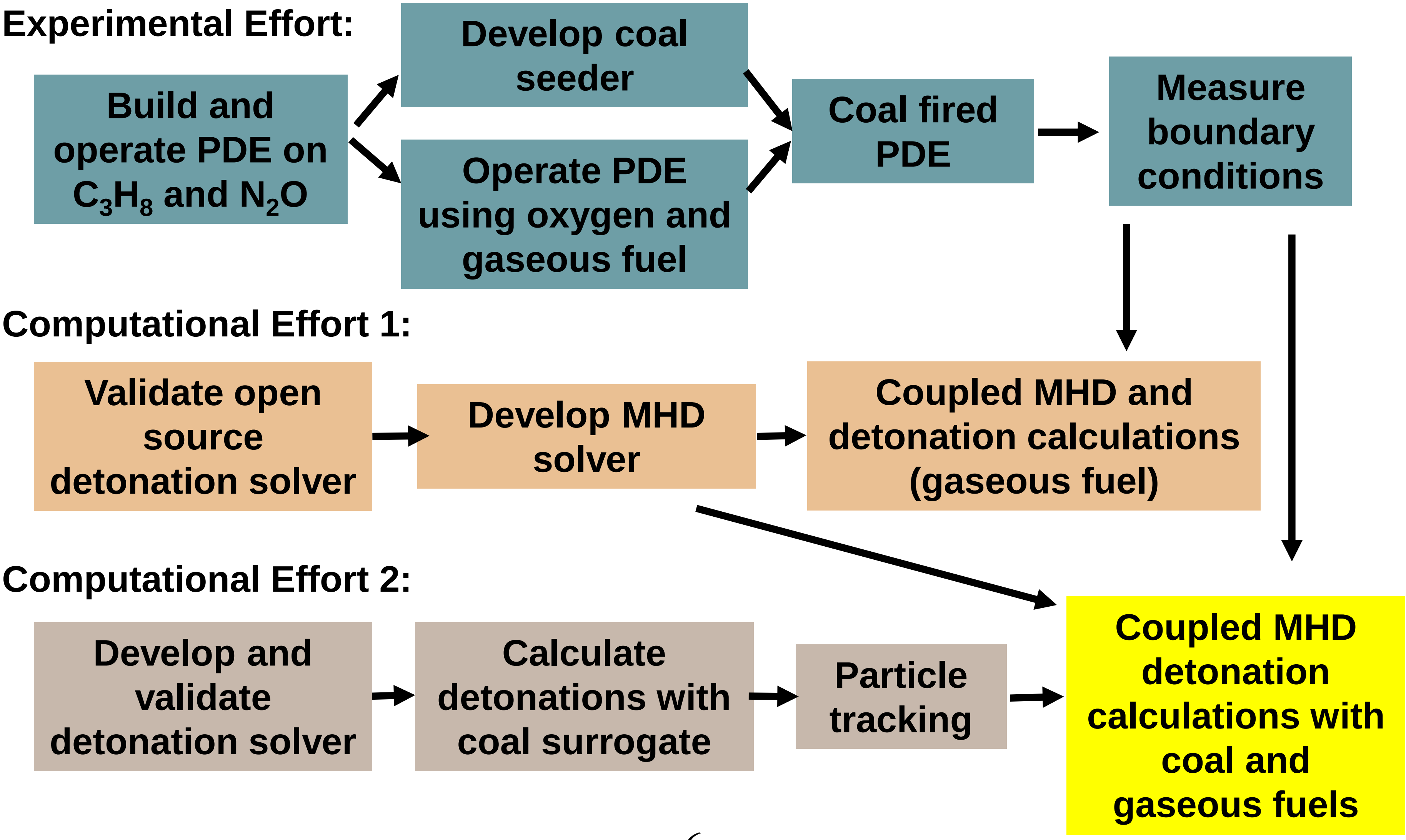
Overall Goal

Develop and evaluate a pulse detonation engine system which can be coupled with a MHD system, and analyze MHD and detonation performance.

Specific Objectives:

1) Design, build, and operate a pulse detonation engine that operates on gaseous or solid fuels with oxygen.
2) Evaluate the operational envelope and performance of the pulse detonation device with both seeded and unseeded flows.
3) Develop and use a numerical design tool to calculate the performance of pulse detonation and coupled detonation-MHD systems.

Progression of Research



Experimental Effort:

Build and operate PDE on C_3H_8 and N_2O

Develop coal seeder

Operate PDE using oxygen and gaseous fuel

Coal fired PDE

Measure boundary conditions

Computational Effort 1:

Validate open source detonation solver

Develop MHD solver

Coupled MHD and detonation calculations (gaseous fuel)

Computational Effort 2:

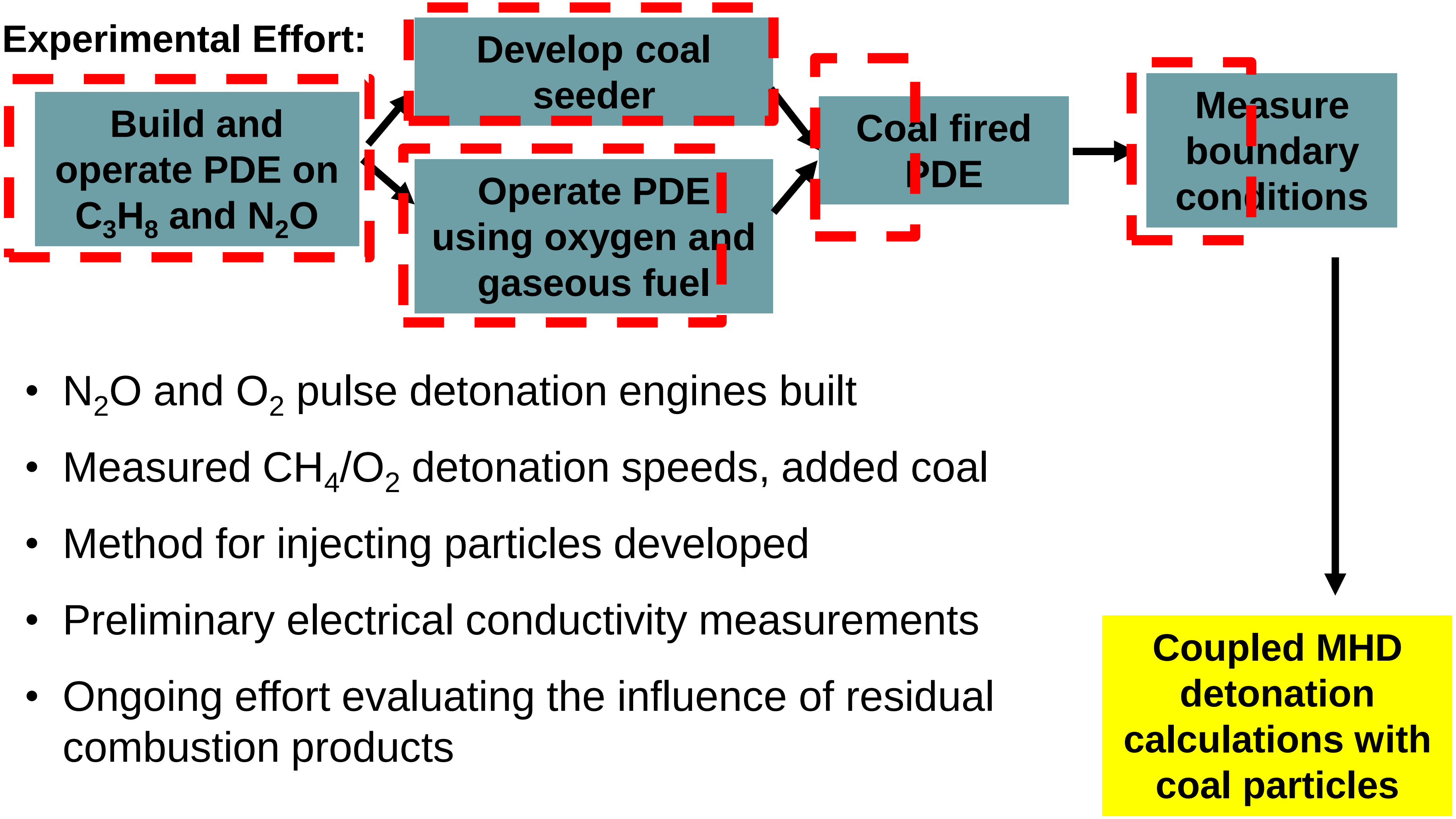
Develop and validate detonation solver

Calculate detonations with coal surrogate

Particle tracking

Coupled MHD detonation calculations with coal and gaseous fuels

Experimental Effort



Experimental Effort:

Build and operate PDE on C_3H_8 and N_2O

Develop coal seeder

Operate PDE using oxygen and gaseous fuel

Coal fired PDE

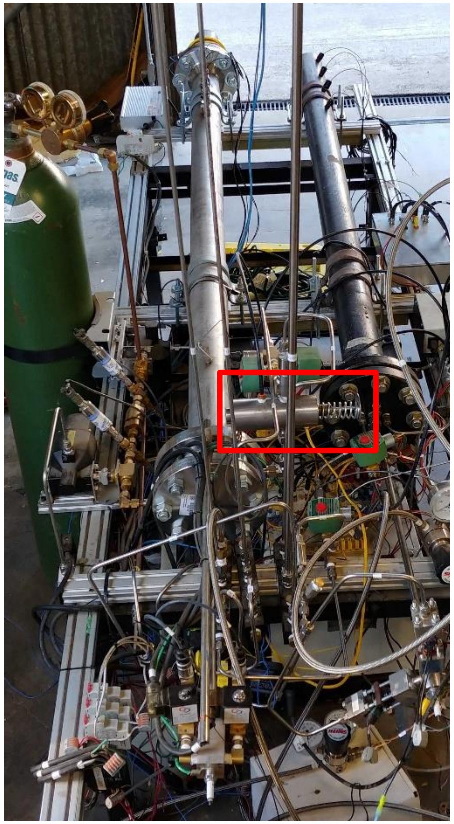
Measure boundary conditions

Coupled MHD detonation calculations with coal particles

- N_2O and O_2 pulse detonation engines built
- Measured CH_4/O_2 detonation speeds, added coal
- Method for injecting particles developed
- Preliminary electrical conductivity measurements
- Ongoing effort evaluating the influence of residual combustion products

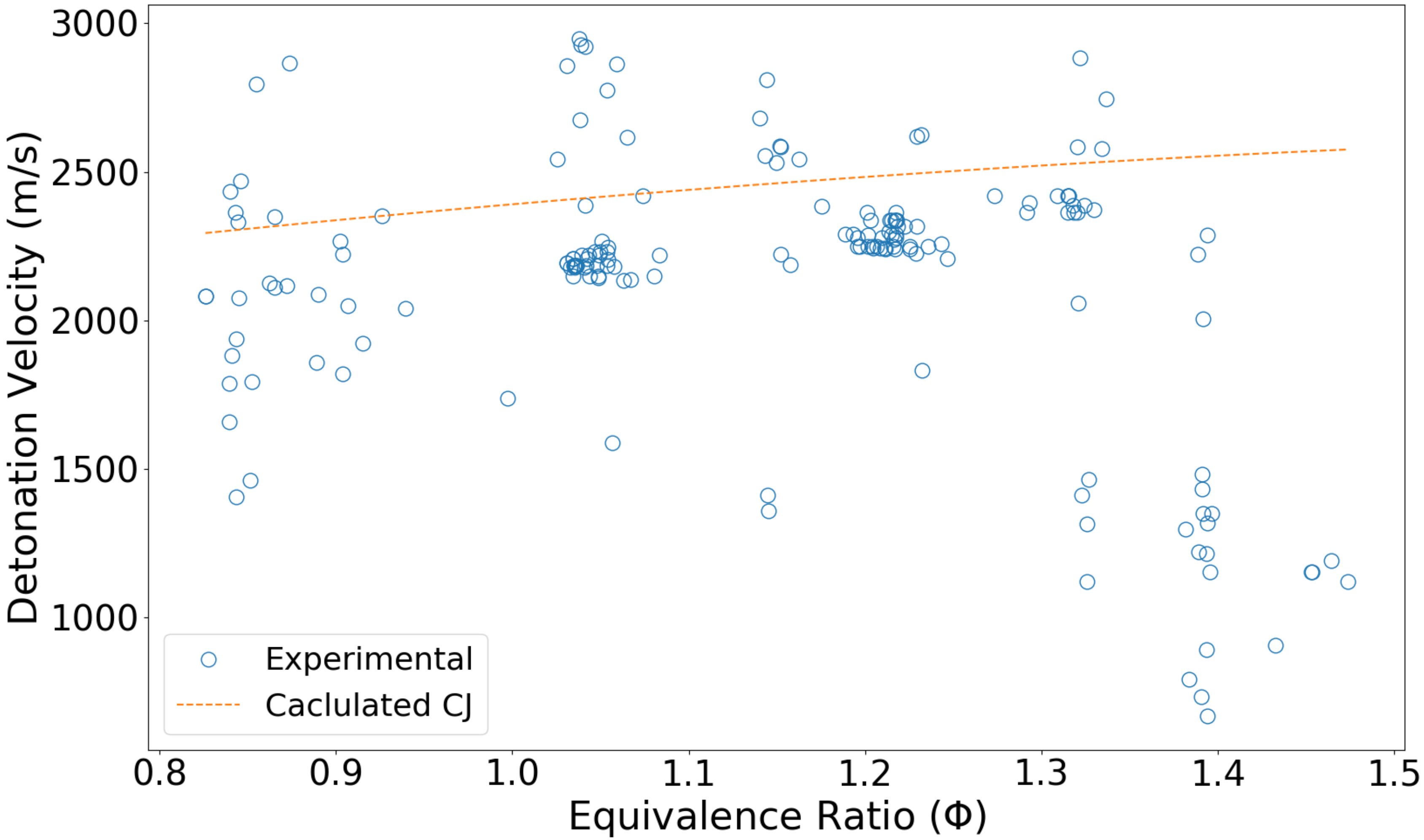
Development of Pulse Detonation System

January 2018

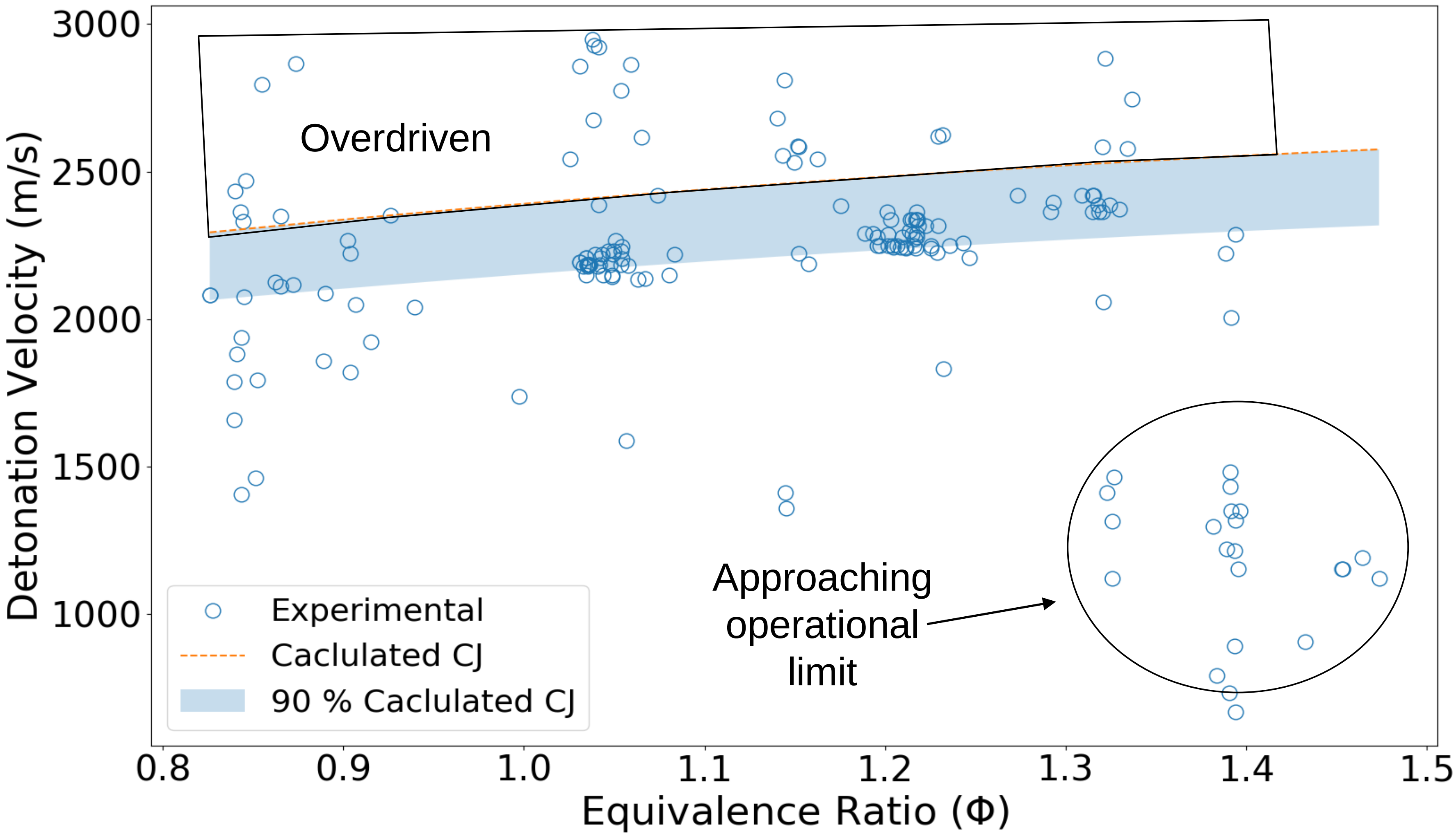


November 2018

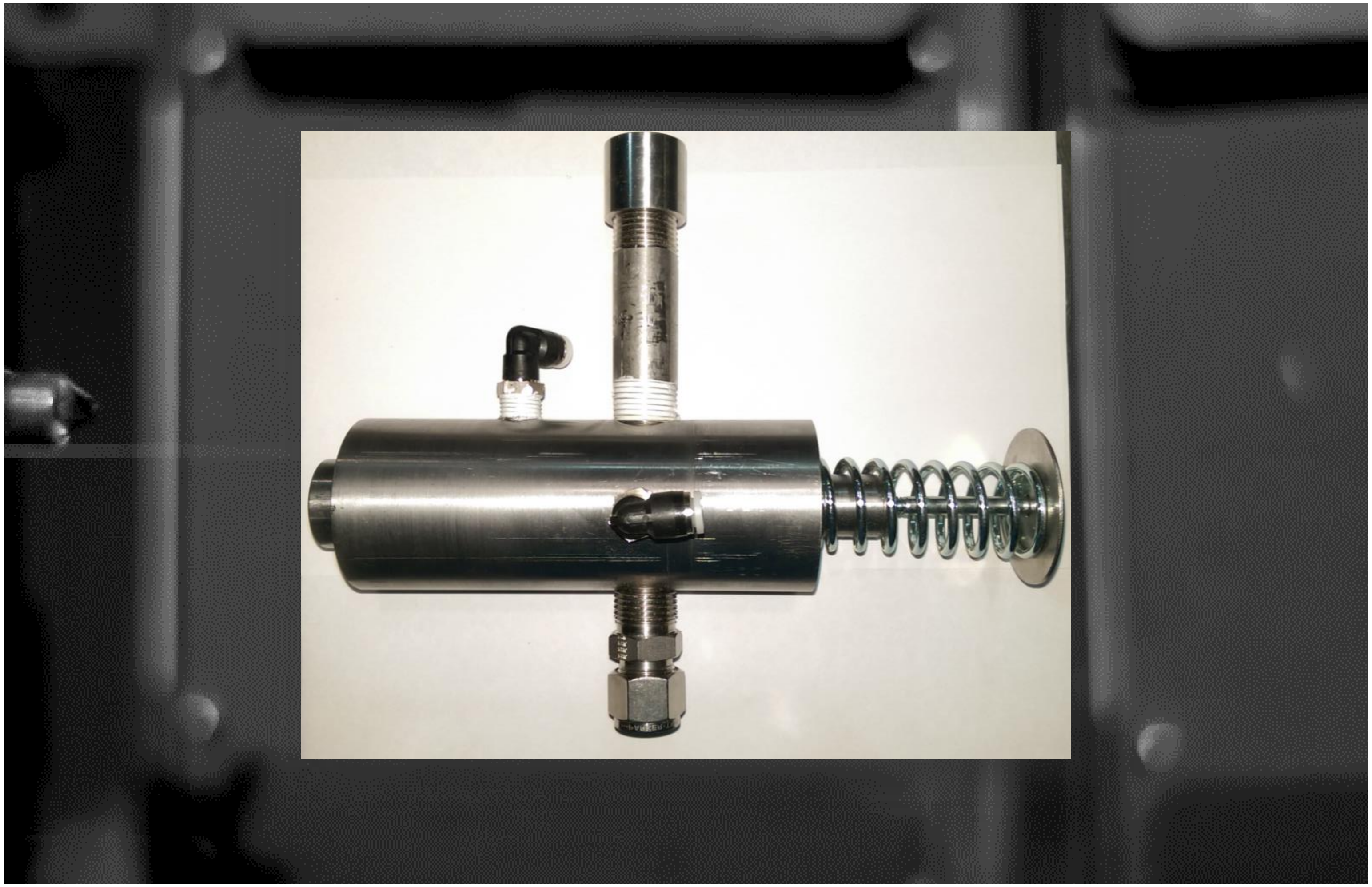
CH_4 – O_2 Detonation Speeds



$CH_4 – O_2$ Detonation Speeds

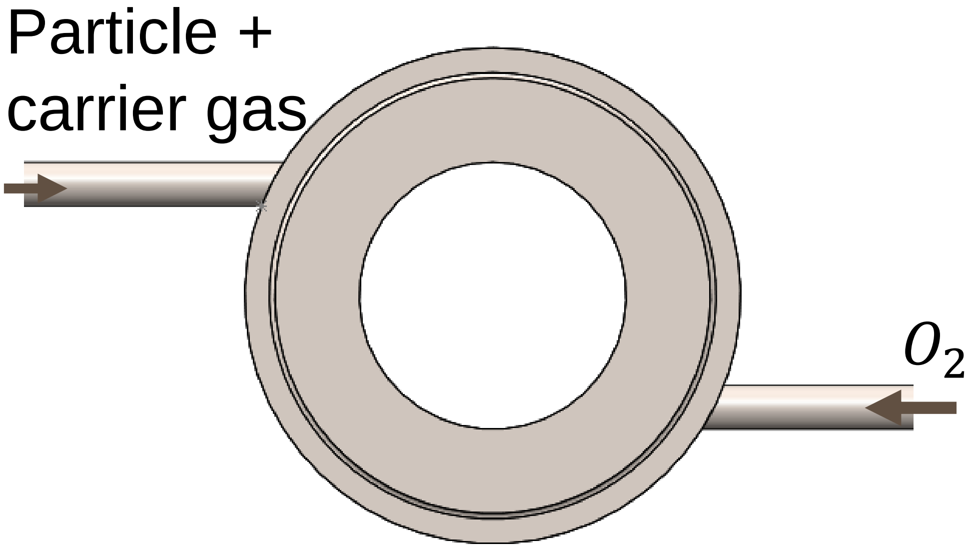


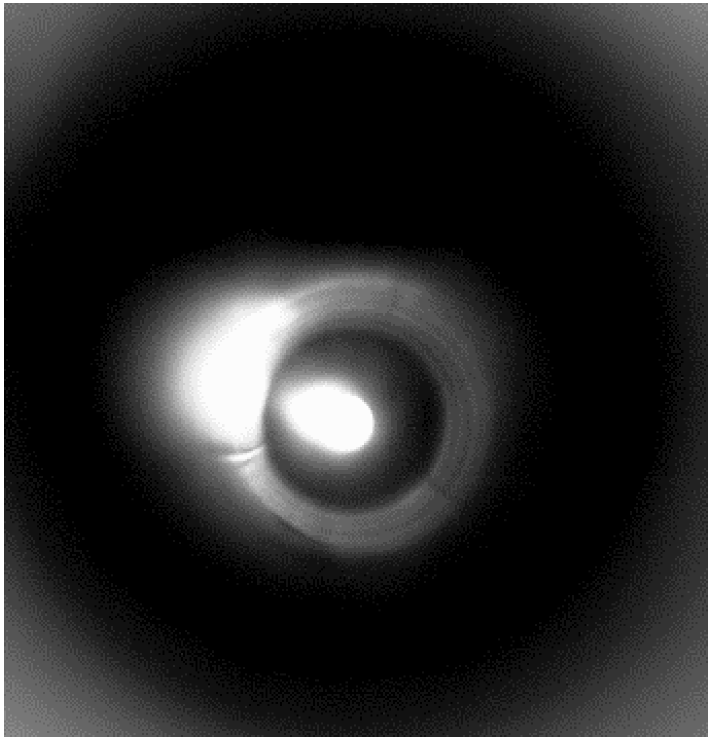
Injection of Seed



High speed video of particulate injection through seeder

Oxygen and Particle Delivery System



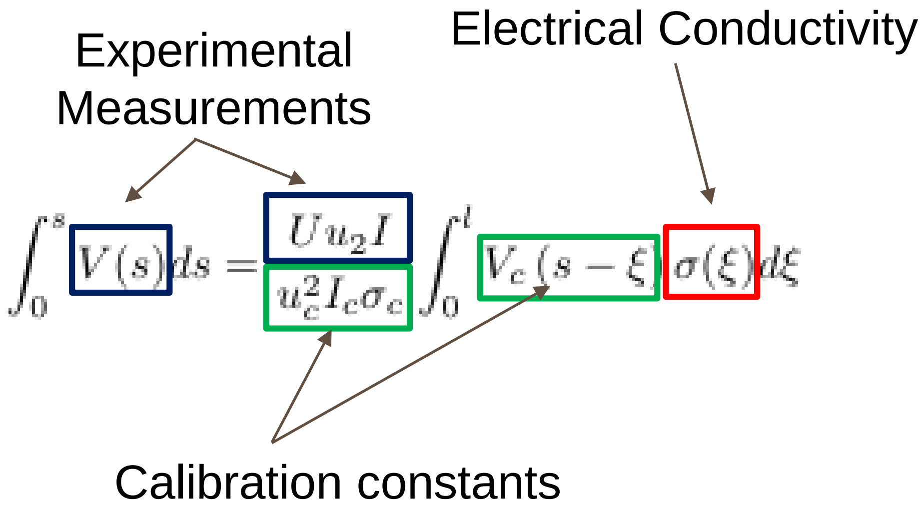


High speed imaging of particle injection

Measuring Electrical Conductivity

$$P \propto \boxed{\sigma} \times V^2 \times B^2$$

- Detonation propagates through magnetic field
- Deflection measured by induced current in search coil
- Conductivity evaluated with relationship:



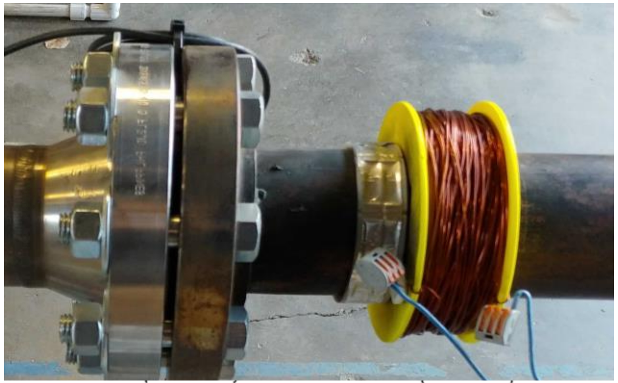
Experimental Measurements

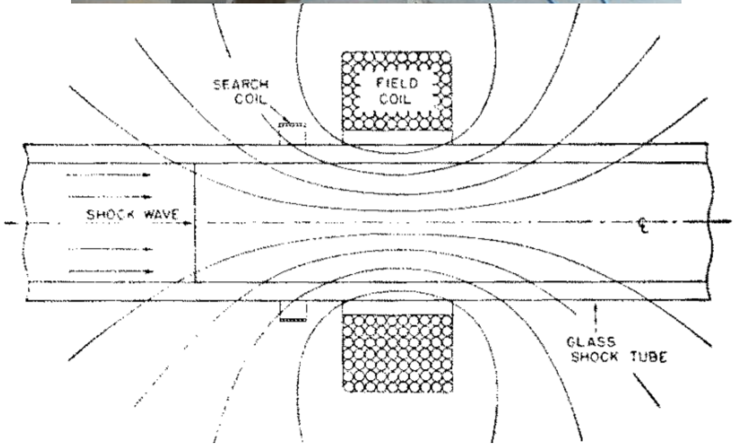
Electrical Conductivity

$$\int_0^s \boxed{V(s)}\,ds = \frac{\boxed{U u_2 I}}{\boxed{u_c^2 I_c \sigma_c}} \int_0^l \boxed{V_c(s-\xi)}\,\boxed{\sigma(\xi)}\,d\xi$$

Calibration constants

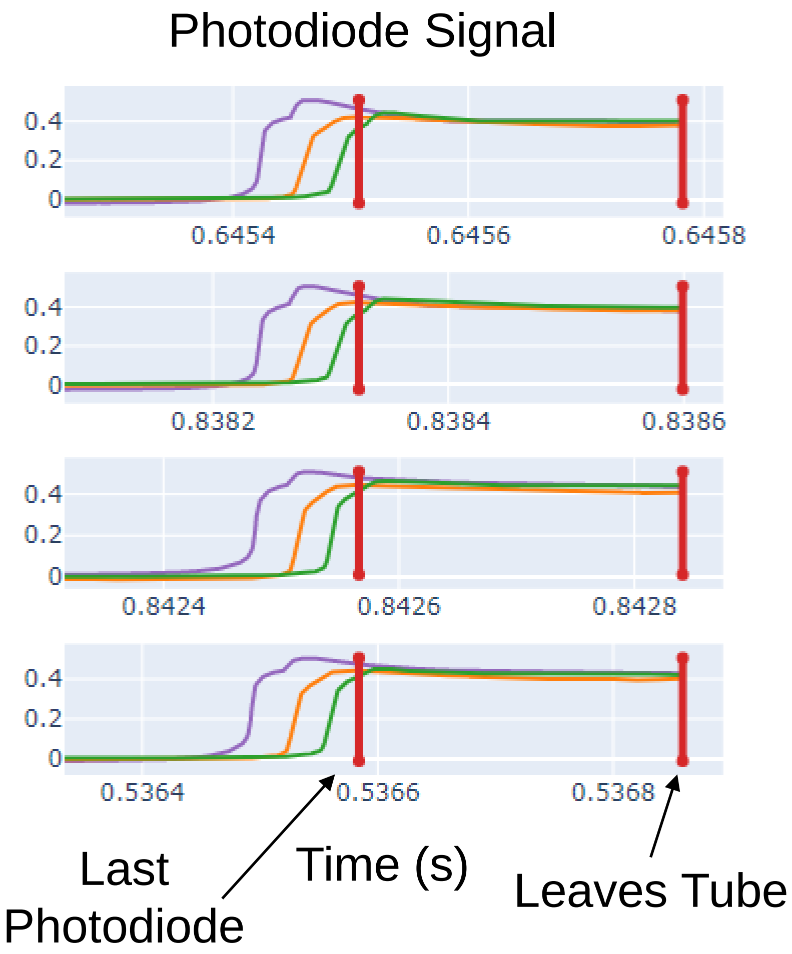
Instrumentation to measure electrical conductivity





Lin et al., Journal of Applied Physics

Electrical Conductivity Signal


Photodiode Signal

Oxy-methane φ≈ 1 for all tests

Progression of Research

Computational Effort 1:

Validate open source detonation solver → **Develop MHD solver** → **Coupled MHD and detonation calculations (gaseous fuel)**

- 2D simulations of detonation through H_2-O_2
- 1D simulations of hydrocarbon detonations
- 1D ionizing H_2-O_2-KOH model has developed and applied
- Riemann solvers initially updated to account for MHD in1D

Coupled MHD detonation calculations with coal particles

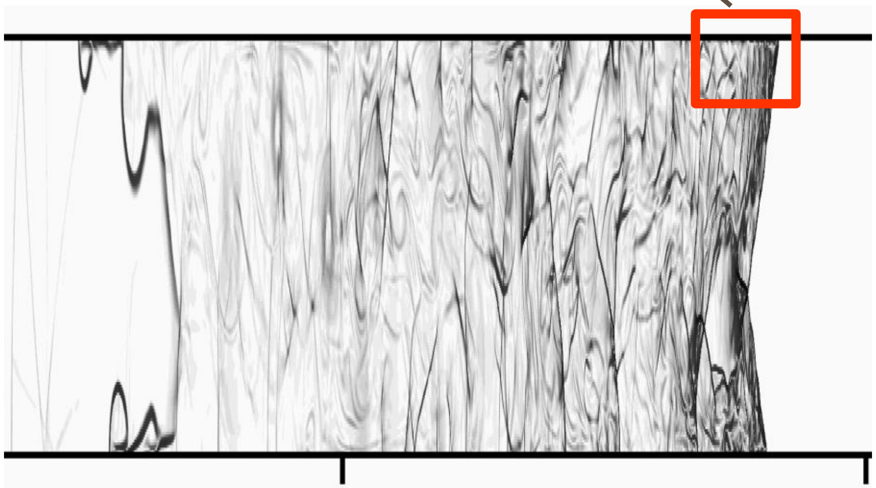
Detonation Solver

- Godonov’s finite volume with Conservation Laws Package (CLAWpack) 5.4.0 (Mandli et al, 2016)

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}\right)$$

- Riemann approximation with Roe averaging and entropy inclusion
- Kinetics handled by Cantera 2.3.0

Cell Width = 3.2 [mm]
Experimental = 2.02 [mm]
(Denisov,1960)



CLAWPack DOI:10.5281/zenodo.262111,URL: http://www.clawpack.org

Cantera DOI:10.5281/zenodo.170284,URL: http://www.cantera.org

Governing Eq. for MHD/Detonation

Mass conservation equation:

$$\frac{\partial}{\partial t}\iint_S \rho dS = -\int_l \rho \boldsymbol{u}\cdot\boldsymbol{n}dl$$

$\boldsymbol{u}$: Gas Velocity ρ: Density p: Pressure

$\boldsymbol{B}$: Magnetic Flux Density $\boldsymbol{J}$: Electric Current Density

E: Total Energy σ: Electrical Conductivity

Momentum conservation equation:

$$\frac{\partial}{\partial t}\iint_S \rho\boldsymbol{u}dS = -\int_l \{\rho\boldsymbol{u}(\boldsymbol{u}\cdot\boldsymbol{n}) + p\boldsymbol{n}\}dl + \int_l \bar{\bar{\tau}}\cdot\boldsymbol{n}dl + \iint_S \boldsymbol{J}\times\boldsymbol{B}dS$$

Total energy conservation equation:

$$\frac{\partial}{\partial t}\iint_S \rho E dS = -\int_l (\rho E\boldsymbol{u}\cdot\boldsymbol{n} + p\boldsymbol{u}\cdot\boldsymbol{n})dl + \int_l (\bar{\bar{\tau}}\cdot\boldsymbol{u})\cdot\boldsymbol{n}dl + \iint_S \left\{\frac{\boldsymbol{J}^2}{\sigma} + \boldsymbol{u}\cdot(\boldsymbol{J}\times\boldsymbol{B})\right\}dS$$

Here,

$$E = \sum_{s=1}^{N_{sp}} Y_s\left(h_{298}{}^{0} + \int_{T'=298\ \mathrm{K}}^{T} c_p{}^{0}\,\mathrm{d}T'\right) - p/\rho + \frac{1}{2}|\boldsymbol{u}|^2$$

Mass conservation equation of Chemical Species:

$$\frac{\partial}{\partial t}\iint_S \rho Y_s dS = -\int_l \rho Y_s\boldsymbol{u}\cdot\boldsymbol{n}dl + \iint_S \rho\dot{Y}_s dS$$

h: Specific Enthalpy

Y_s: Mass Concentration

$\dot{Y}_s$: Mass Production Rate

c_p: Specific Heat at Constant Pressure

Charge Neutrality Equation

$$\frac{Y_e}{m_e} = \sum_i \frac{Y_{ion}}{m_{ion}}$$

Governing Equations in Electrodynamics

Generalized Ohm's Law

$$\boldsymbol{j} = \sigma(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B}) - \frac{\beta}{|\boldsymbol{B}|}\boldsymbol{j} \times \boldsymbol{B}$$

Steady Maxwell Equations

$$\nabla \times \boldsymbol{E} = \boldsymbol{0}$$

$$\nabla \cdot \boldsymbol{j} = 0$$

$\boldsymbol{j}$: Electric Current Density $\boldsymbol{E}$: Electric Field $\boldsymbol{u}$: Gas Velocity $\boldsymbol{B}$: Magnetic Flux Density

Electrical Conductivity $\sigma = \frac{e^2 n_e}{m_e \sum_{i=1}^{N_{sp}} \nu_{ei}}$

Hall Parameter $\beta = \frac{e|\boldsymbol{B}|}{m_e \sum_{i=1}^{N_{sp}} \nu_{ei}}$

Collision Frequency of Electron with Species $\nu_{ei} = n_i Q_{ei} c_e$

e: Elementary Charge

n_e: Electron Number Density

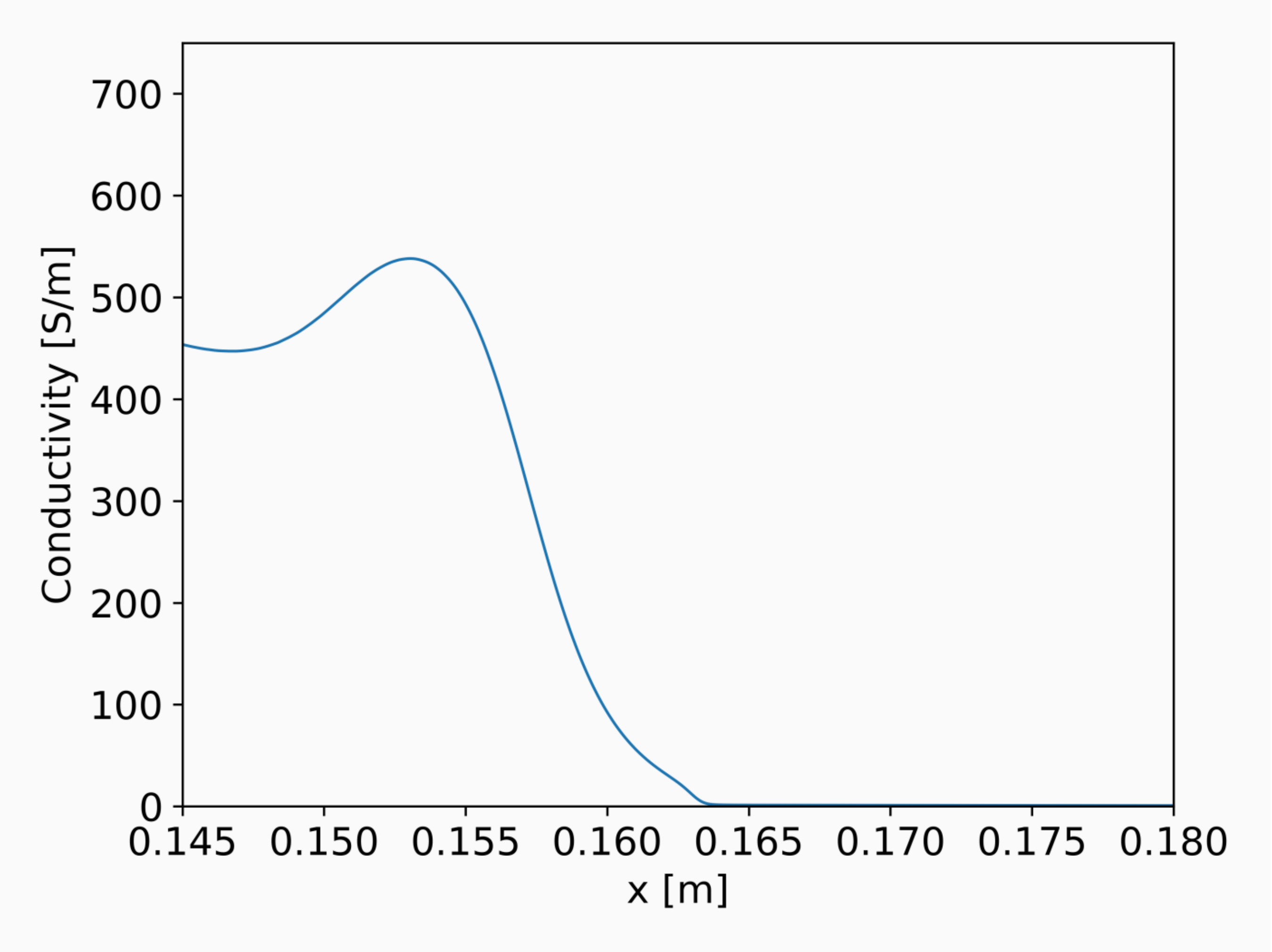
m_e: Electron Mass

n_i: Species Number Density

Q_{ei}: Electron Collision Cross Section with Species

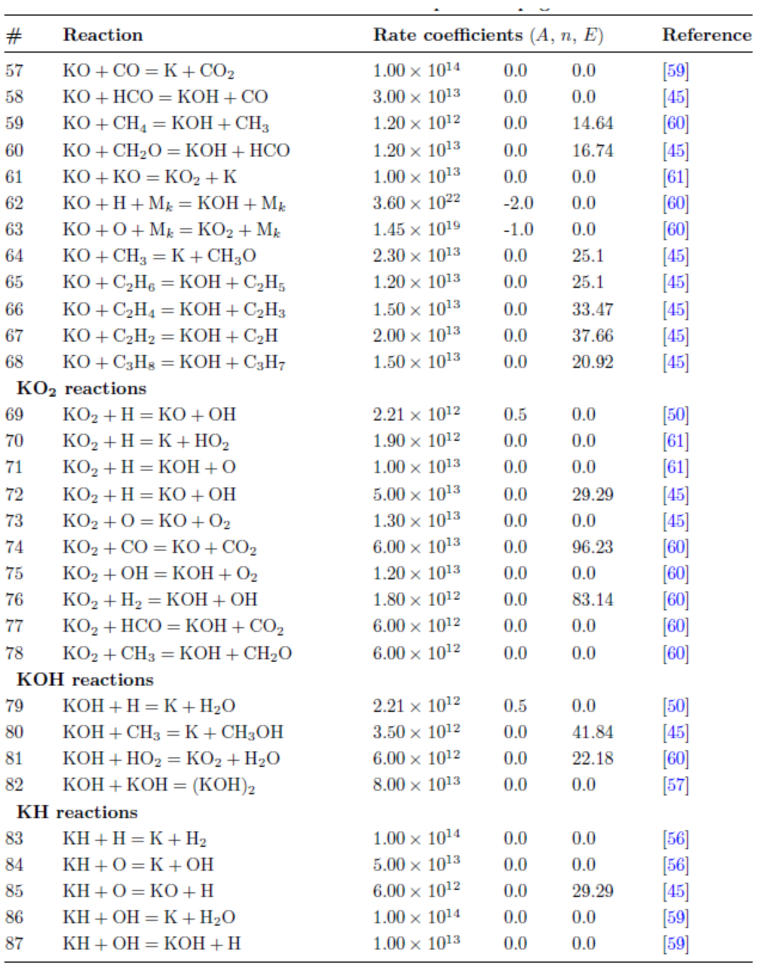
c_e: Electron Mean Thermal Speed

Electrical Conductivity

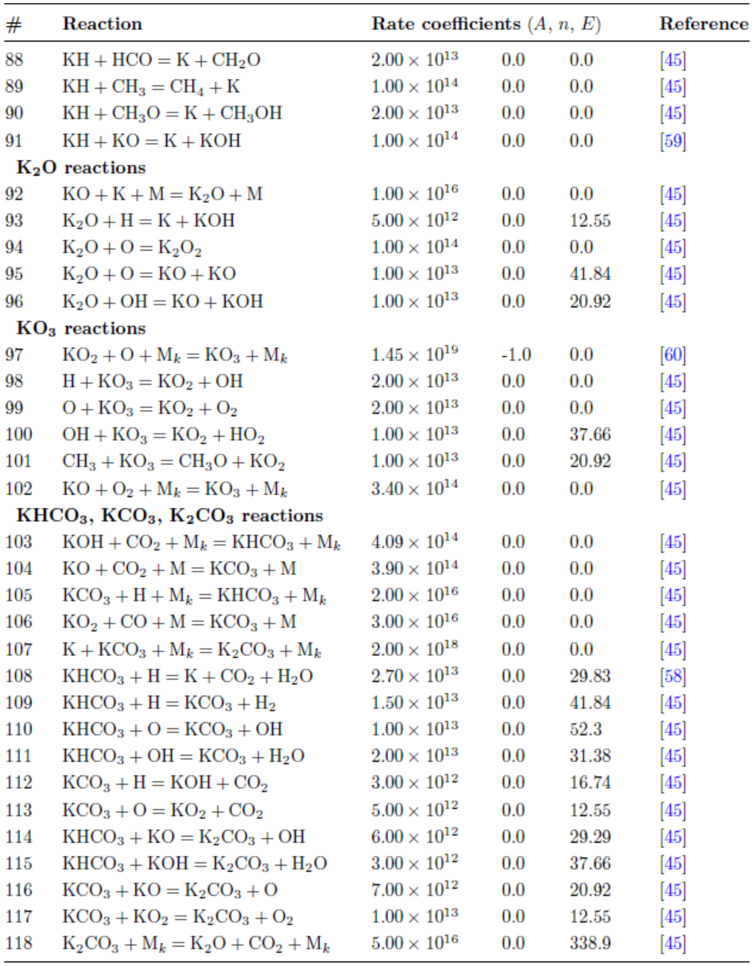


Calculated electrical conductivity

Ionization Mechanism



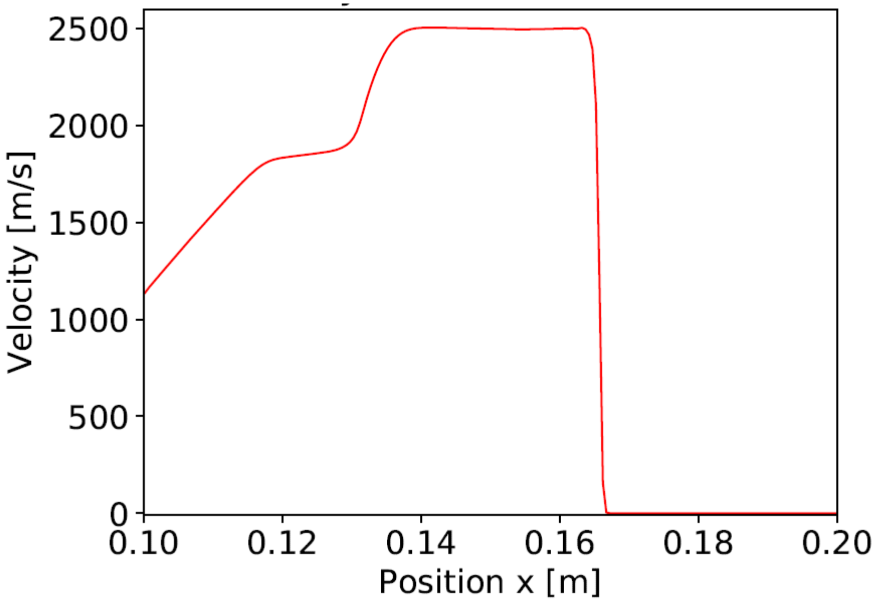
#	Reaction	Rate coefficients (A, n, E)			Reference
57	$KO + CO = K + CO_2$	1.00×10^{14}	0.0	0.0	[59]
58	$KO + HCO = KOH + CO$	3.00×10^{13}	0.0	0.0	[45]
59	$KO + CH_4 = KOH + CH_3$	1.20×10^{12}	0.0	14.64	[60]
60	$KO + CH_2O = KOH + HCO$	1.20×10^{13}	0.0	16.74	[45]
61	$KO + KO = KO_2 + K$	1.00×10^{13}	0.0	0.0	[61]
62	$KO + H + M_k = KOH + M_k$	3.60×10^{22}	-2.0	0.0	[60]
63	$KO + O + M_k = KO_2 + M_k$	1.45×10^{19}	-1.0	0.0	[60]
64	$KO + CH_3 = K + CH_3O$	2.30×10^{13}	0.0	25.1	[45]
65	$KO + C_2H_6 = KOH + C_2H_5$	1.20×10^{13}	0.0	25.1	[45]
66	$KO + C_2H_4 = KOH + C_2H_3$	1.50×10^{13}	0.0	33.47	[45]
67	$KO + C_2H_2 = KOH + C_2H$	2.00×10^{13}	0.0	37.66	[45]
68	$KO + C_3H_8 = KOH + C_3H_7$	1.50×10^{13}	0.0	20.92	[45]
KO_2 reactions					
69	$KO_2 + H = KO + OH$	2.21×10^{12}	0.5	0.0	[50]
70	$KO_2 + H = K + HO_2$	1.90×10^{12}	0.0	0.0	[61]
71	$KO_2 + H = KOH + O$	1.00×10^{13}	0.0	0.0	[61]
72	$KO_2 + H = KO + OH$	5.00×10^{13}	0.0	29.29	[45]
73	$KO_2 + O = KO + O_2$	1.30×10^{13}	0.0	0.0	[45]
74	$KO_2 + CO = KO + CO_2$	6.00×10^{13}	0.0	96.23	[60]
75	$KO_2 + OH = KOH + O_2$	1.20×10^{13}	0.0	0.0	[60]
76	$KO_2 + H_2 = KOH + OH$	1.80×10^{12}	0.0	83.14	[60]
77	$KO_2 + HCO = KOH + CO_2$	6.00×10^{12}	0.0	0.0	[60]
78	$KO_2 + CH_3 = KOH + CH_2O$	6.00×10^{12}	0.0	0.0	[60]
KOH reactions					
79	$KOH + H = K + H_2O$	2.21×10^{12}	0.5	0.0	[50]
80	$KOH + CH_3 = K + CH_3OH$	3.50×10^{12}	0.0	41.84	[45]
81	$KOH + HO_2 = KO_2 + H_2O$	6.00×10^{12}	0.0	22.18	[60]
82	$KOH + KOH = (KOH)_2$	8.00×10^{13}	0.0	0.0	[57]
KH reactions					
83	$KH + H = K + H_2$	1.00×10^{14}	0.0	0.0	[56]
84	$KH + O = K + OH$	5.00×10^{13}	0.0	0.0	[56]
85	$KH + O = KO + H$	6.00×10^{12}	0.0	29.29	[45]
86	$KH + OH = K + H_2O$	1.00×10^{14}	0.0	0.0	[59]
87	$KH + OH = KOH + H$	1.00×10^{13}	0.0	0.0	[59]



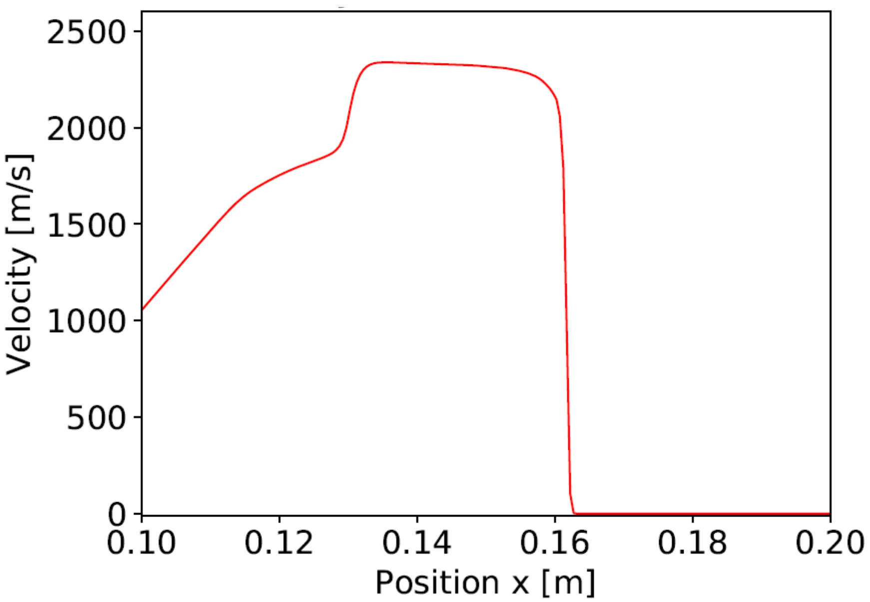
#	Reaction	Rate coefficients (A, n, E)			Reference
88	$KH + HCO = K + CH_2O$	2.00×10^{13}	0.0	0.0	[45]
89	$KH + CH_3 = CH_4 + K$	1.00×10^{14}	0.0	0.0	[45]
90	$KH + CH_3O = K + CH_3OH$	2.00×10^{13}	0.0	0.0	[45]
91	$KH + KO = K + KOH$	1.00×10^{14}	0.0	0.0	[59]
K_2O reactions					
92	$KO + K + M = K_2O + M$	1.00×10^{16}	0.0	0.0	[45]
93	$K_2O + H = K + KOH$	5.00×10^{12}	0.0	12.55	[45]
94	$K_2O + O = K_2O_2$	1.00×10^{14}	0.0	0.0	[45]
95	$K_2O + O = KO + KO$	1.00×10^{13}	0.0	41.84	[45]
96	$K_2O + OH = KO + KOH$	1.00×10^{13}	0.0	20.92	[45]
KO_3 reactions					
97	$KO_2 + O + M_k = KO_3 + M_k$	1.45×10^{19}	-1.0	0.0	[60]
98	$H + KO_3 = KO_2 + OH$	2.00×10^{13}	0.0	0.0	[45]
99	$O + KO_3 = KO_2 + O_2$	2.00×10^{13}	0.0	0.0	[45]
100	$OH + KO_3 = KO_2 + HO_2$	1.00×10^{13}	0.0	37.66	[45]
101	$CH_3 + KO_3 = CH_3O + KO_2$	1.00×10^{13}	0.0	20.92	[45]
102	$KO + O_2 + M_k = KO_3 + M_k$	3.40×10^{14}	0.0	0.0	[45]
$KHCO_3$, KCO_3, K_2CO_3 reactions					
103	$KOH + CO_2 + M_k = KHCO_3 + M_k$	4.09×10^{14}	0.0	0.0	[45]
104	$KO + CO_2 + M = KCO_3 + M$	3.90×10^{14}	0.0	0.0	[45]
105	$KCO_3 + H + M_k = KHCO_3 + M_k$	2.00×10^{16}	0.0	0.0	[45]
106	$KO_2 + CO + M = KCO_3 + M$	3.00×10^{16}	0.0	0.0	[45]
107	$K + KCO_3 + M_k = K_2CO_3 + M_k$	2.00×10^{18}	0.0	0.0	[45]
108	$KHCO_3 + H = K + CO_2 + H_2O$	2.70×10^{13}	0.0	29.83	[58]
109	$KHCO_3 + H = KCO_3 + H_2$	1.50×10^{13}	0.0	41.84	[45]
110	$KHCO_3 + O = KCO_3 + OH$	1.00×10^{13}	0.0	52.3	[45]
111	$KHCO_3 + OH = KCO_3 + H_2O$	2.00×10^{13}	0.0	31.38	[45]
112	$KCO_3 + H = KOH + CO_2$	3.00×10^{12}	0.0	16.74	[45]
113	$KCO_3 + O = KO_2 + CO_2$	5.00×10^{12}	0.0	12.55	[45]
114	$KHCO_3 + KO = K_2CO_3 + OH$	6.00×10^{12}	0.0	29.29	[45]
115	$KHCO_3 + KOH = K_2CO_3 + H_2O$	3.00×10^{12}	0.0	37.66	[45]
116	$KCO_3 + KO = K_2CO_3 + O$	7.00×10^{12}	0.0	20.92	[45]
117	$KCO_3 + KO_2 = K_2CO_3 + O_2$	1.00×10^{13}	0.0	12.55	[45]
118	$K_2CO_3 + M_k = K_2O + CO_2 + M_k$	5.00×10^{16}	0.0	338.9	[45]

Zaiger, 2019

Detonation Speeds with 0.01% K_2CO_3



Ionization chemistry inactive



Ionization chemistry active

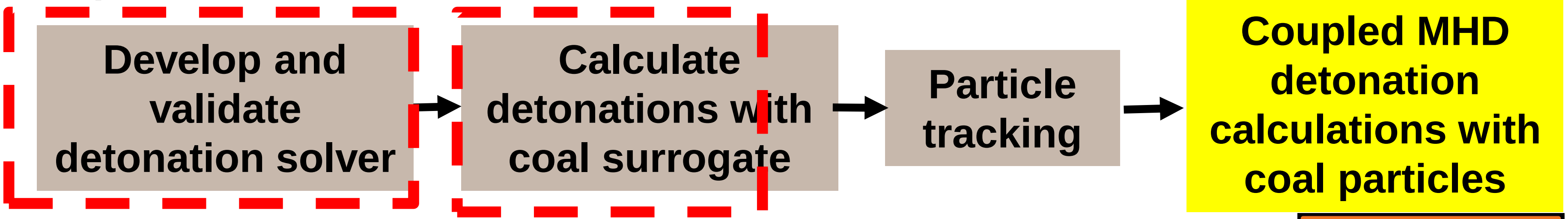
- Up to an 8% decrease in the detonation speed
- Decrease in power

[Zaiger, 2019]

Progression of Research

- Multi-species & multi-step reacting flow CESE solver
- Fully implicit & dual time stepping source term for stiff chemistry
- Oxy-fuel detonation simulation
- 2D solver framework

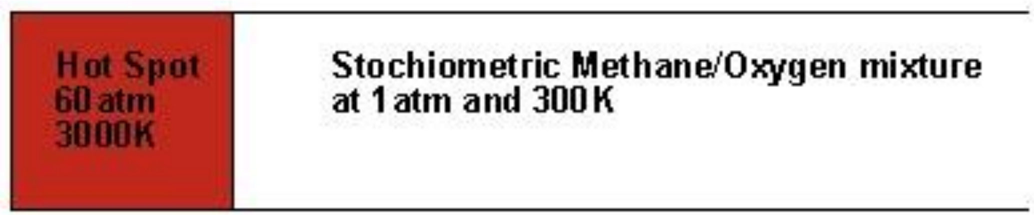
Computational Effort 2:



Develop and validate detonation solver → **Calculate detonations with coal surrogate** → **Particle tracking** → **Coupled MHD detonation calculations with coal particles**

CH_4–O_2 Detonation: JLR mechanism

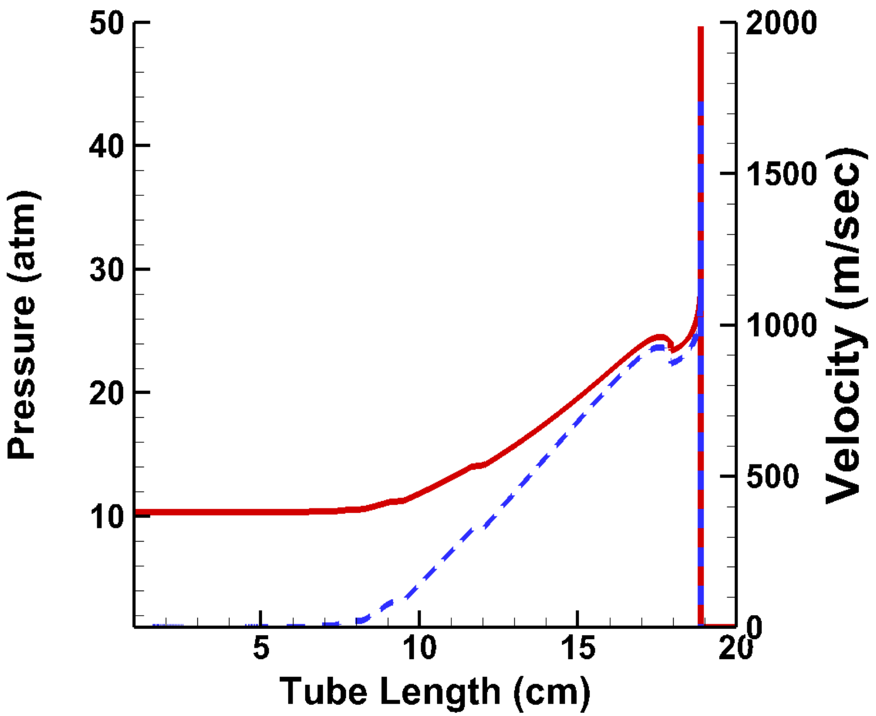
- Detonation propagation in CH_4/O_2 mixtures
- Modified JL-R mechanism
  - Chemical kinetics for a multistep, Arrhenius-type chemical reaction for nine species: CH_4, O_2, H_2, CO_2, CO, OH, H, O and H_2O adopted

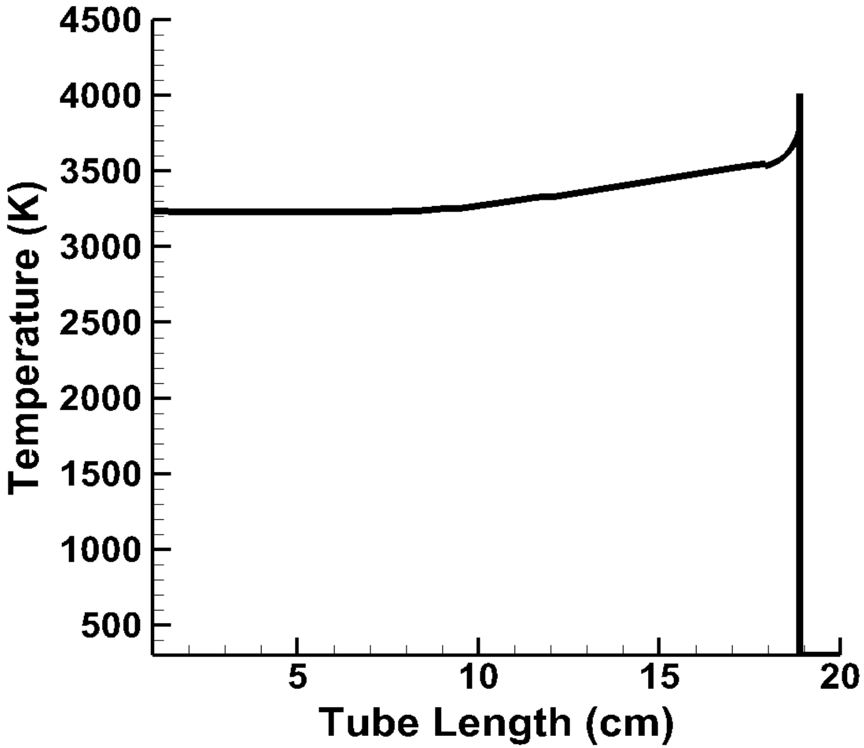


No	Reaction	Reaction Kinetics
1	$CH_4 + 0.5O_2 \longrightarrow CO + 2H_2$	$r_1 = 3.06.10^{11} \exp\left(\frac{-30000}{RT}\right)[CH_4]^{0.5}[O_2]^{1.30}$
2	$CH_4 + H_2O \longrightarrow CO + 3H_2$	$r_2 = 3.84.10^{9} \exp\left(\frac{-30000}{RT}\right)[CH_4][H_2O]$
3	$CO + H_2O \rightleftharpoons CO_2 + H_2$	$r_3 = 2.01.10^{9} \exp\left(\frac{-20000}{RT}\right)[CO][H_2O]$
4	$H_2 + 0.5O_2 \rightleftharpoons H_2O$	$r_4 = 8.03.10^{16} T^{-1} \exp\left(\frac{-40000}{RT}\right)[H_2]^{0.3}[O_2]^{1.55}$
5	$O_2 \rightleftharpoons 2O$	$r_5 = 1.5.10^{9} \exp\left(\frac{-113000}{RT}\right)[O_2]$
6	$H_2O \rightleftharpoons H + OH$	$r_6 = 2.3.10^{22} T^{-3} \exp\left(\frac{-120000}{RT}\right)[H_2O]$

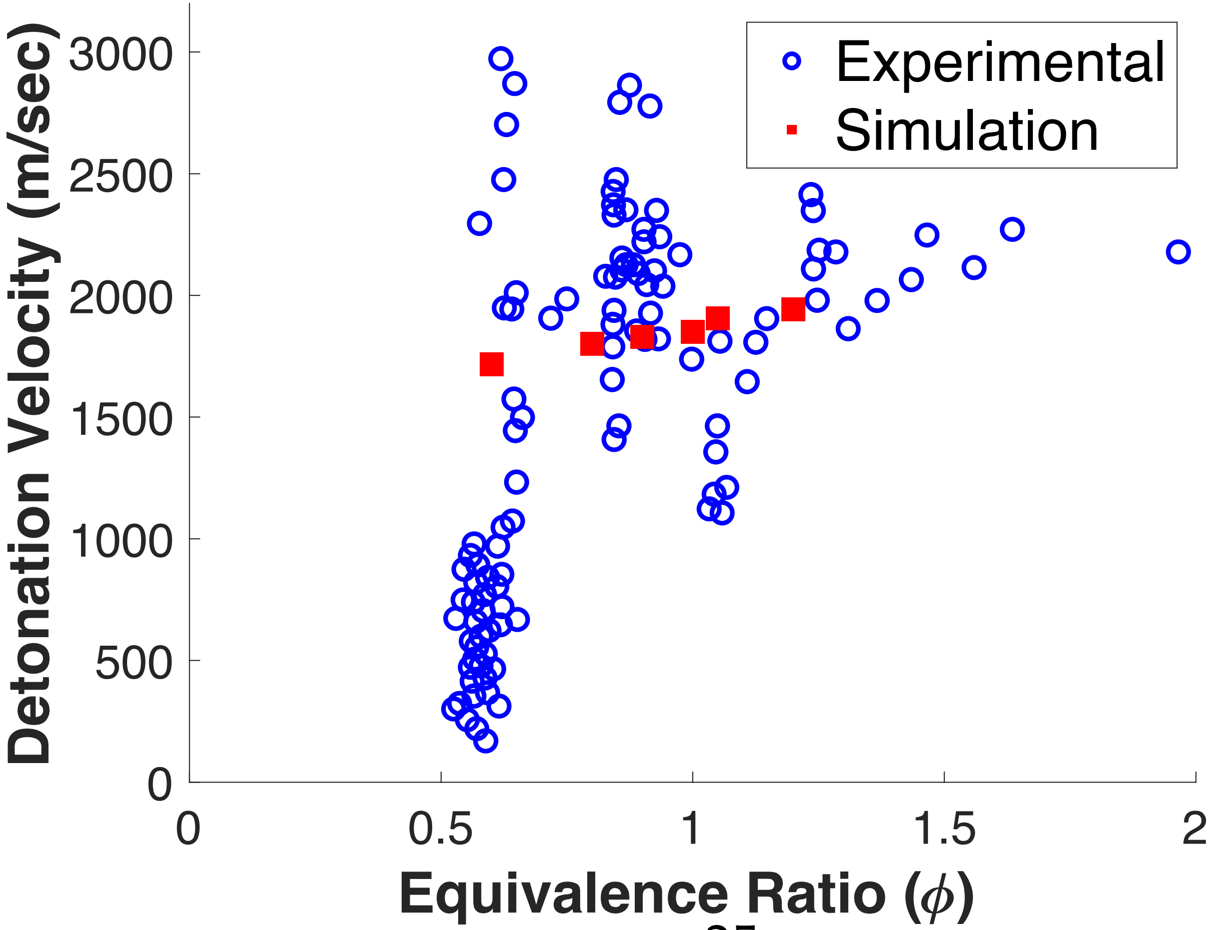
- Radical dissociation accounted in modified JL-R mechanism
- Critical in appropriately limiting heat release during oxy-combustion, thereby predicting detonation temperature and velocity accurately

CH_4–O_2 Detonation (Φ=1)



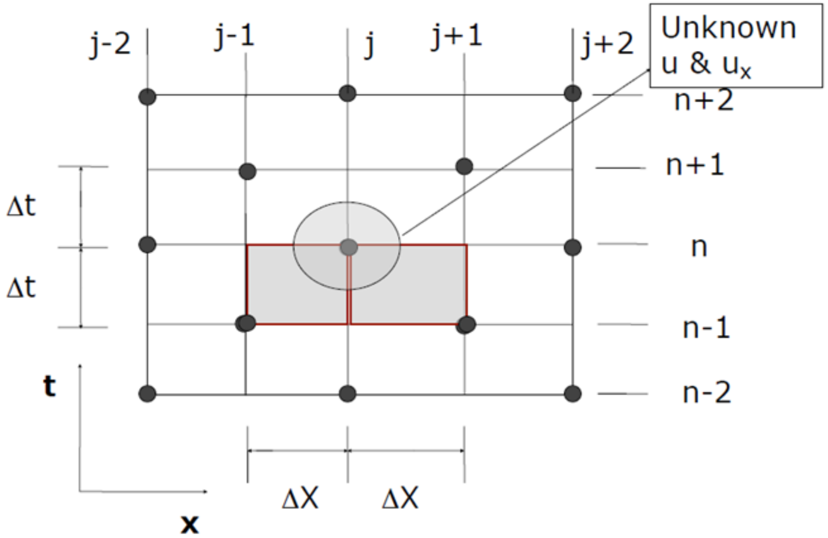


CH_4–O_2 Detonation: Comparison with Experimental Data

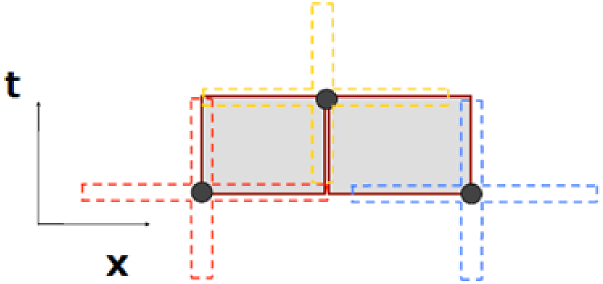


Conservation Element Solution Element (CESE) Numerical Method Basics

- Flux conservation over discretized space-time domain – not just along spatial domain as in traditional FV method
- Staggered integration volumes (CE) and solution volumes (SE)
  - Riemann solution not needed
- Genuine multi-dimensional formulation
  - No dimensional/directional splitting necessary
  - Applicable to unstructured grids
- Non-dissipative baseline "a-scheme"
  - Numerical dissipation added as necessary



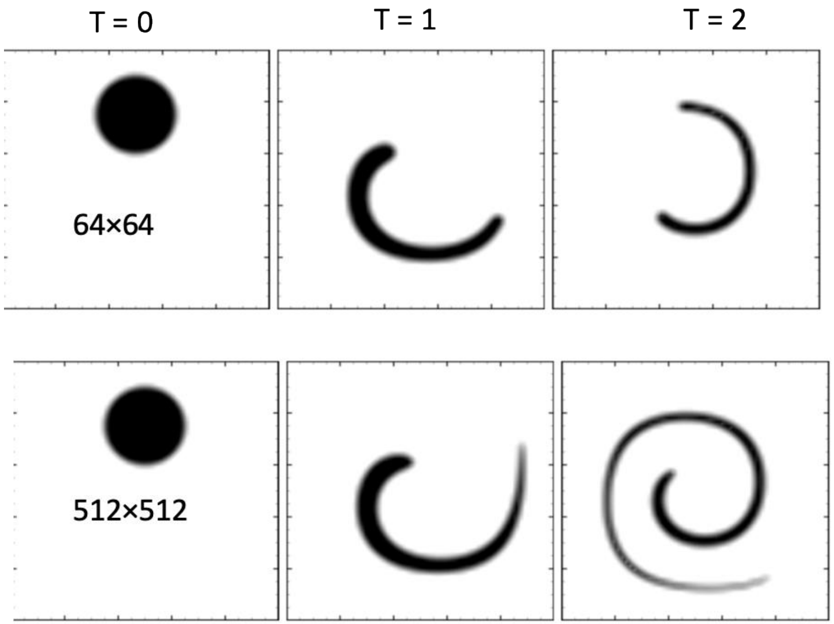
1D CESE Space-Time Staggered Grid*



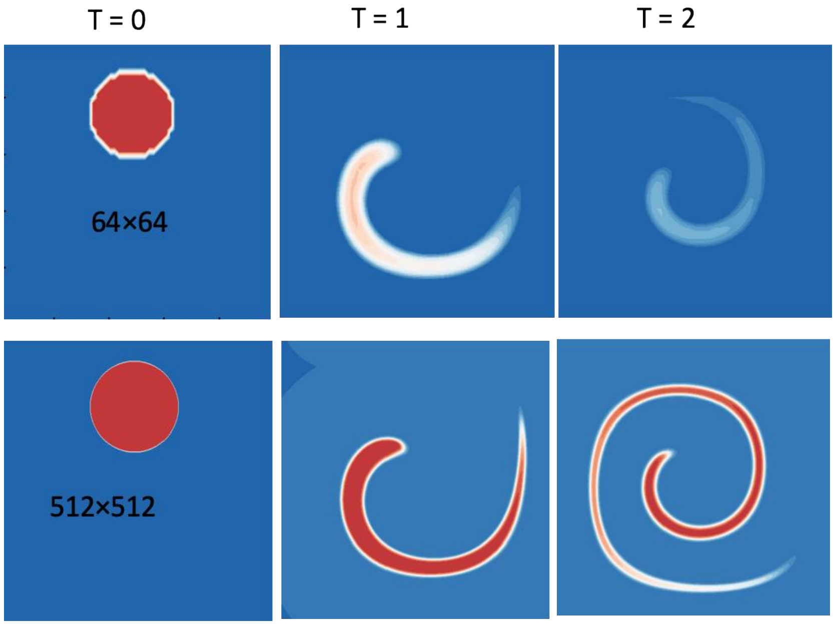
CE (non-overlapping rectangular regions) & SE (dotted lines) *

Vortex in a Box

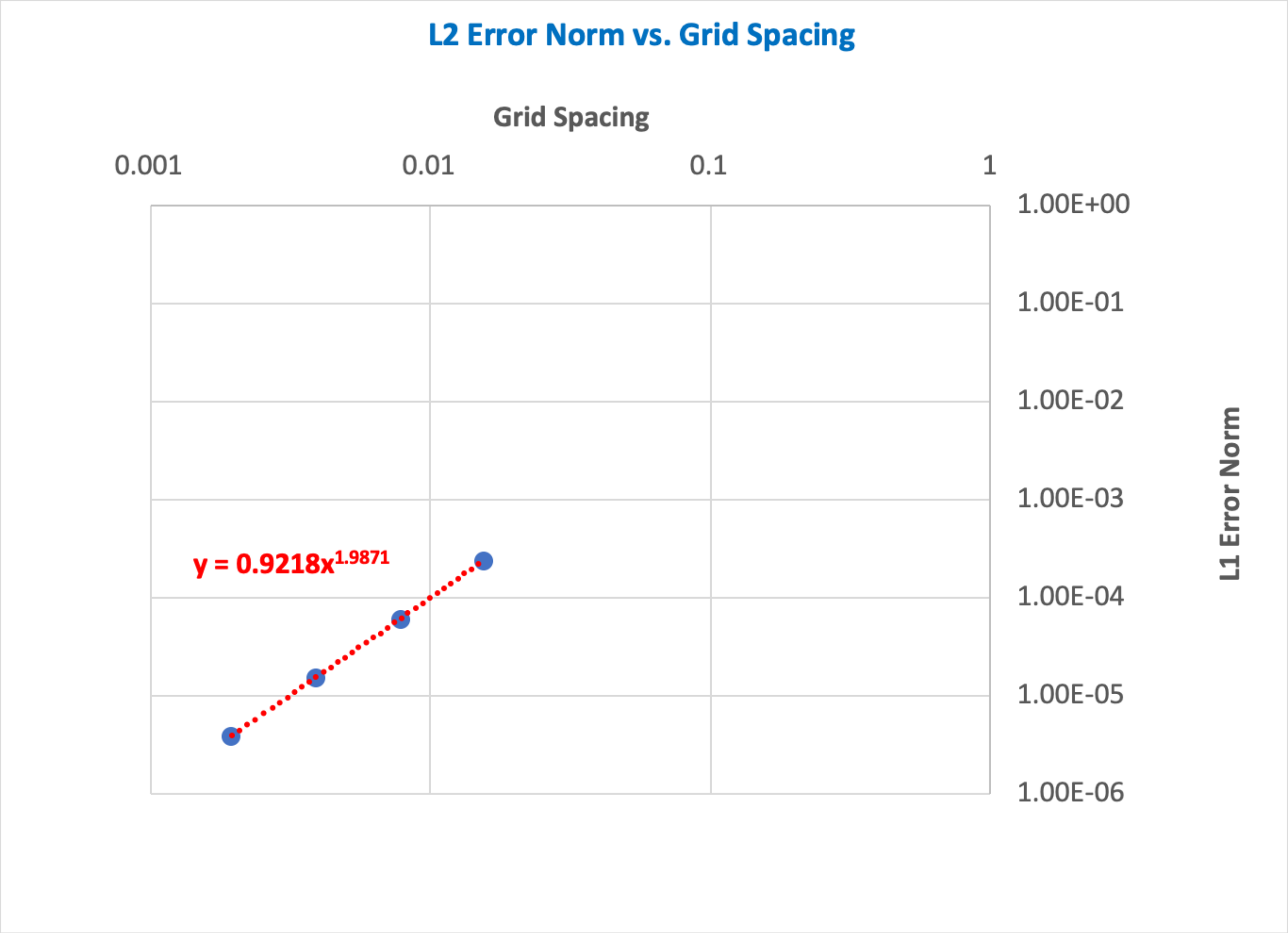
Hermann, 2005



Current 2D CE/SE Solver



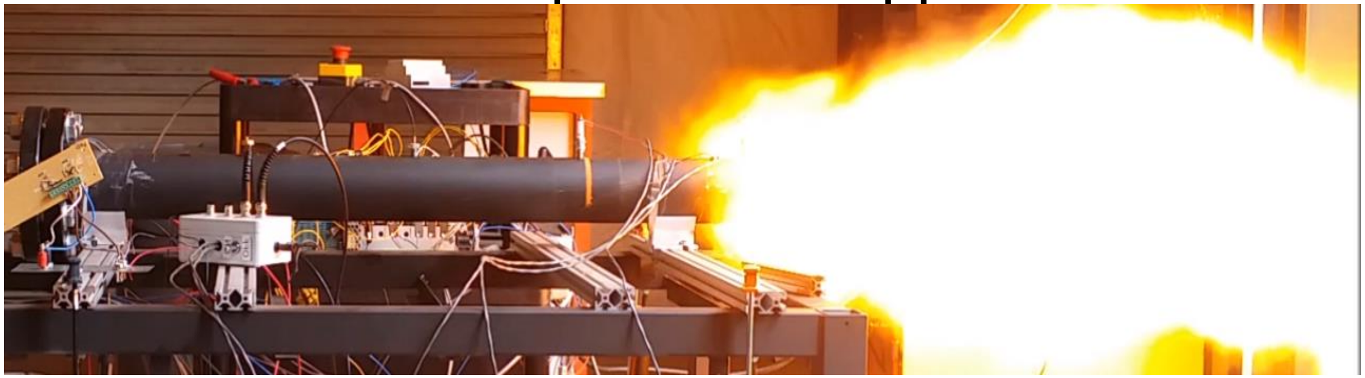
Evaluation of CESE 2D Solver



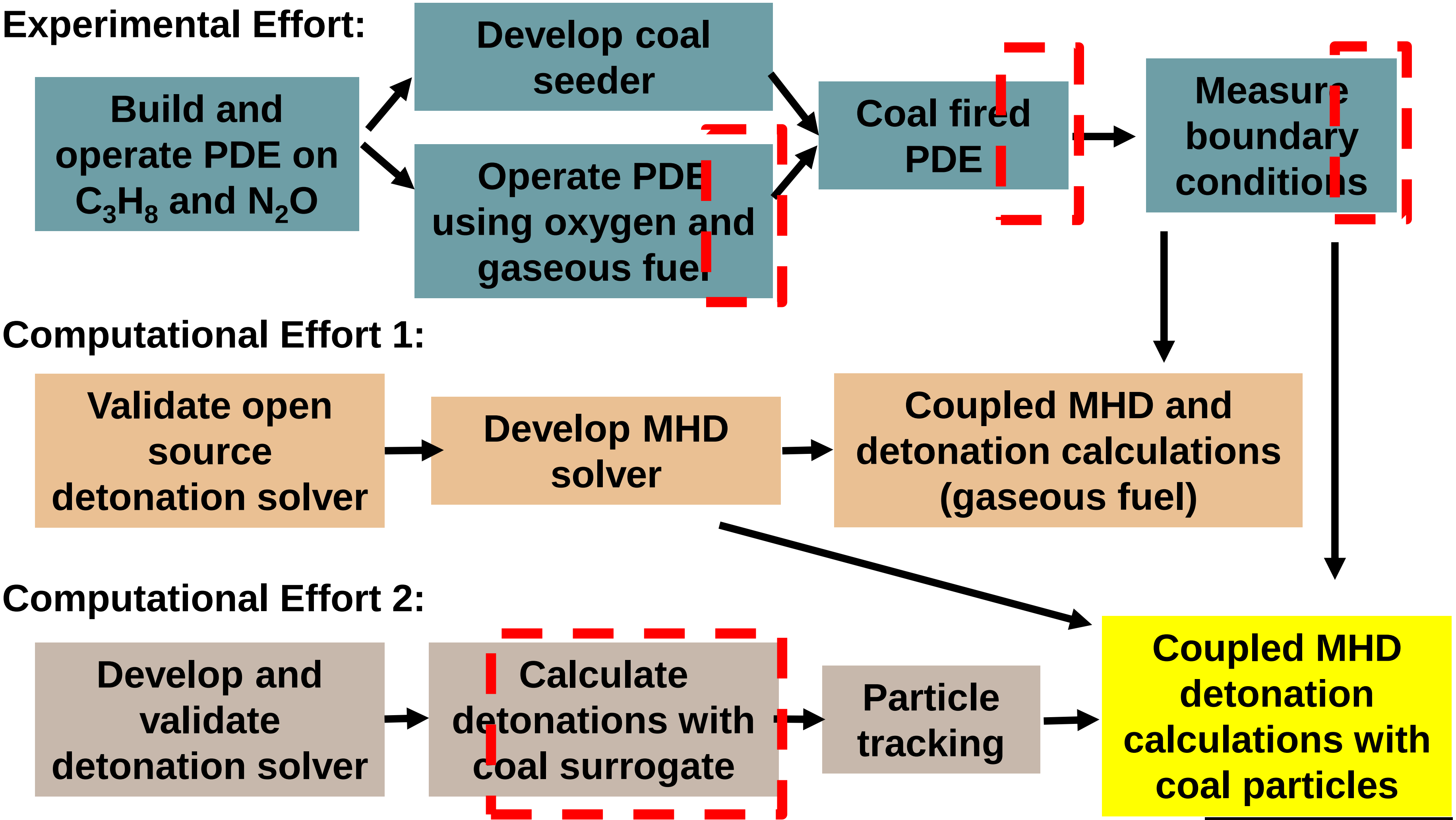
Key Findings

$$P \propto \sigma \times V^2 \times B^2$$

1) Particle seeder developed for unsteady detonations
2) Data collected for CH_4-O_2 detonations
3) Electrical conductivity measurements being collected, preliminary results indicate seeding needed
4) Ionization chemistry of seed particles reduces detonation speed
5) Detonation solver developed for oxygen-fuel combustion
6) Residual combustion products suppress detonations



Future Work



Experimental Effort:

Build and operate PDE on C_3H_8 and N_2O

Develop coal seeder

Operate PDE using oxygen and gaseous fuel

Coal fired PDE

Measure boundary conditions

Computational Effort 1:

Validate open source detonation solver

Develop MHD solver

Coupled MHD and detonation calculations (gaseous fuel)

Computational Effort 2:

Develop and validate detonation solver

Calculate detonations with coal surrogate

Particle tracking

Coupled MHD detonation calculations with coal particles

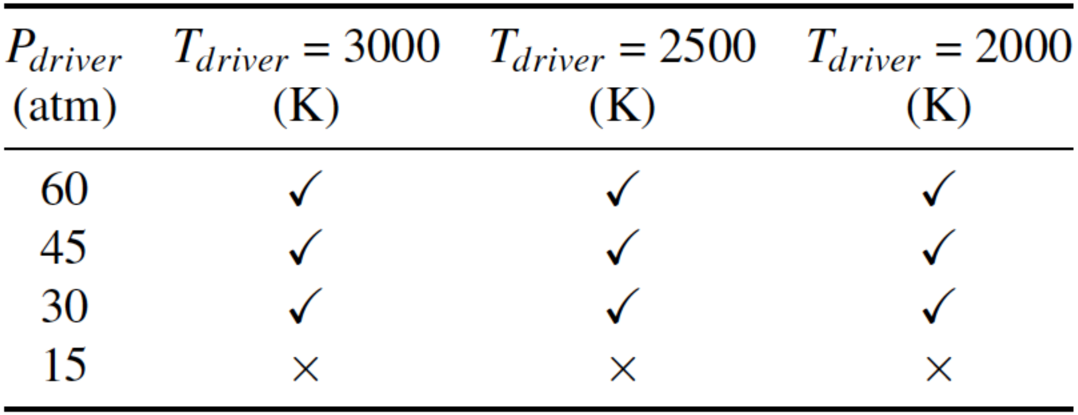
CIRE Lab

NRG

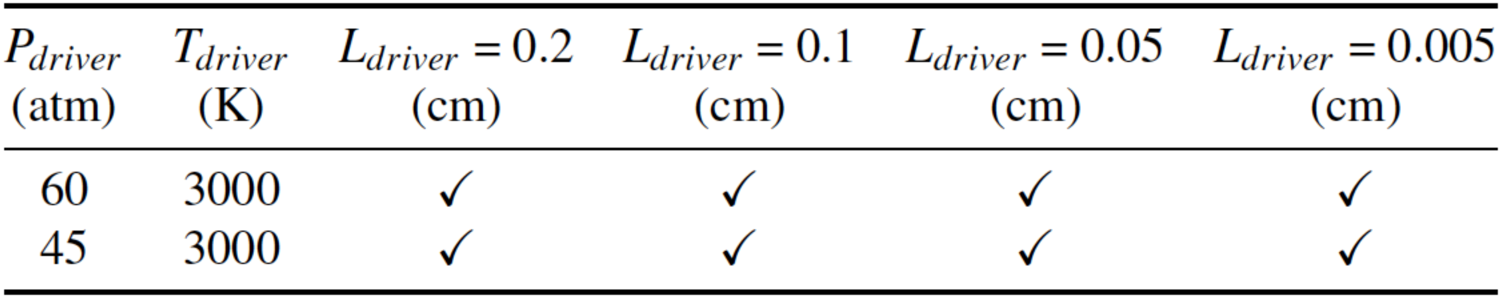
PROPULSION LABORATORY

Detonation Initiation Studies

- Effect of driver shock pressure and temperature on detonation initiation was studied to establish operational envelope for CH_4–O_2 detonations



P_{driver} (atm)	$T_{driver} = 3000$ (K)	$T_{driver} = 2500$ (K)	$T_{driver} = 2000$ (K)
60	✓	✓	✓
45	✓	✓	✓
30	✓	✓	✓
15	×	×	×



P_{driver} (atm)	T_{driver} (K)	$L_{driver} = 0.2$ (cm)	$L_{driver} = 0.1$ (cm)	$L_{driver} = 0.05$ (cm)	$L_{driver} = 0.005$ (cm)
60	3000	✓	✓	✓	✓
45	3000	✓	✓	✓	✓

Detonations with Coal

Without Coal

With Coal

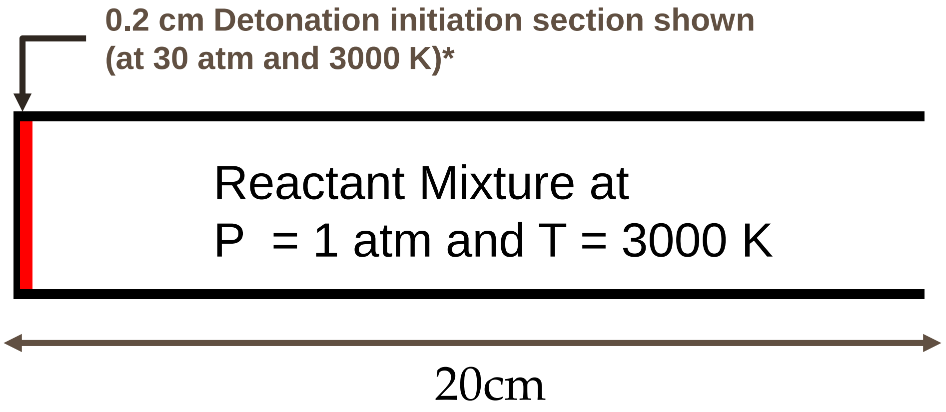
23k frames per second with 0.3 μs integration time

CESE Solver Validation (ZND Detonation)

- **ZND Detonation Propagation in a Tube**
- Arrhenius-type chemical reaction for two species (reactant & product)

$$Reactant(R) \rightarrow Product(P) + heat\ release(q)$$

- 20cm tube filled with premixed stochiometric H_2/O_2 reactant mixture
- 0.2 cm spark region placed near closed head end to initiate detonation
- Validated against ZND theory and with Wu, 2002

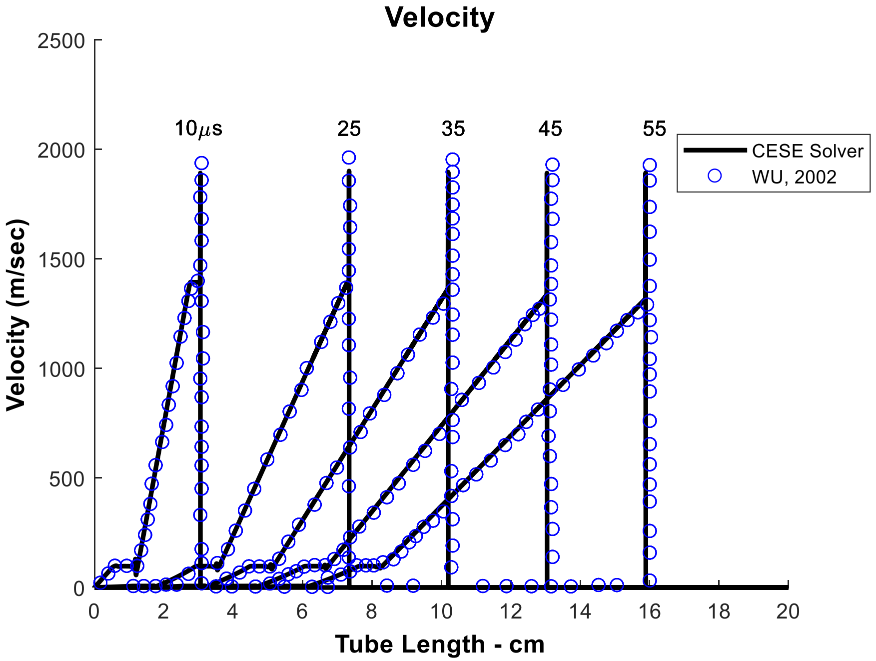


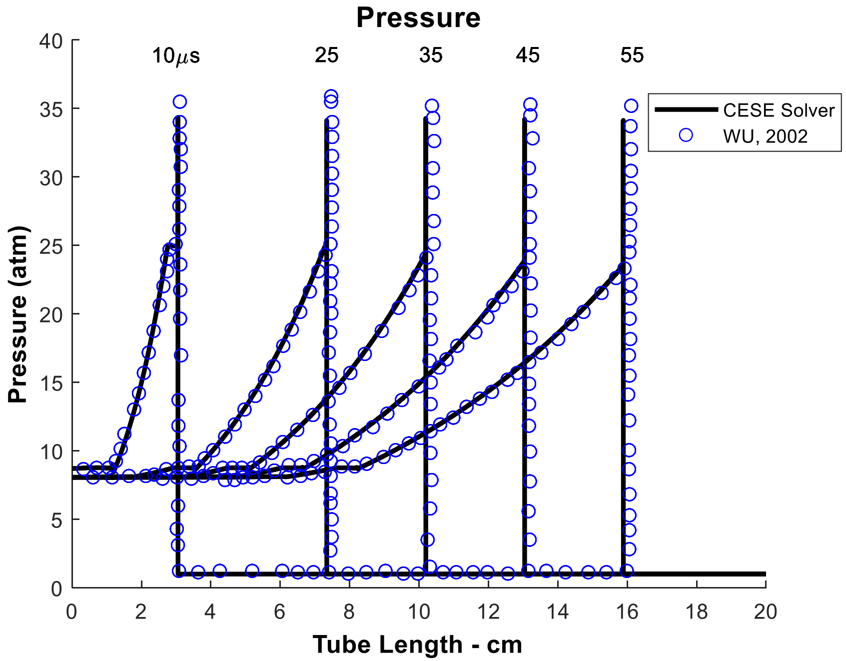
0.2 cm Detonation initiation section shown (at 30 atm and 3000 K)*

Reactant Mixture at
P = 1 atm and T = 3000 K

20cm

CESE Solver Validation (ZND Detonation)





Source	P_s (atm)	P_2 (atm)	T_2 (K)	P_3 (atm)
CESE Solver	34.24	22.1	3745	8.06
Wu, 2002	36.0	22.0	3736	8.05
ZND Theory	42.9	22.1	3743	8.06

$P_s = Von\ Neumann\ pressure\ spike$

$P_2, T_2 = CJ\ pressure$ and temperature

$P_3 = Head\ end\ pressure$

H_2-Air and CH_4–O_2 Detonation comparison

- Temperature higher in CH_4-O_2 detonation than H_2-Air detonation
  - Consistent with expectation of oxy-fuel combustion.
  - Higher temperature and high detonation wave velocity should result in more power extraction for MHD unit
- WD scheme over predicts combustion temperature as result of not accounting for dissociation reactions
- At temperatures higher than 2500 K (which are very common in oxy-fuel combustion), the CO-CO_2 equilibrium is in favor of CO

Governing Equations for 1D Reacting Flows

Conservation equations for chemically reacting system involving N_s species

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}=S$$

$$Q=\begin{bmatrix}\rho\\ \rho u\\ \rho e_t\\ C_1\\ C_2\\ \vdots\\ C_{N_{s-1}}\end{bmatrix},\ \mathrm{E}=\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho u\left(e_t+\frac{p}{\rho}\right)\\ uC_1\\ uC_2\\ \vdots\\ uC_{N_{s-1}}\end{bmatrix},\ \mathrm{S}=\begin{bmatrix}0\\ 0\\ 0\\ \dot{\omega}_1\\ \dot{\omega}_2\\ \vdots\\ \dot{\omega}_{N_{s-1}}\end{bmatrix}$$

$$e_t=e+\frac{1}{2}u^2$$

$$\rho e=\ \sum_{i=1}^{N_s}C_i\left(\int_{T_{ref}}^{T}C_{pi}dt+\ h_{fi}^{0}\right)-p$$

$$\dot{\omega}_j=\ MW_j\sum_{i=}^{N_R}(\nu_{ij}''-\nu_{ij}')\left(k_{fi}\prod_{l=1}^{N_s}n_l^{\nu_{ij}''}-k_{bi}\prod_{l=1}^{N_s}n_l^{\nu_{ij}'}\right)$$

$\rho = density$

$u = velocity$

$C_i = species\ mass\ concentration$

$p = pressure$

$\dot{\omega}_i = mass\ production\ rate\ of\ ith$

$species\ per\ unit\ volume$

$n_j = molar\ concentration\ of\ species\ j$

$k_{fi} = forward\ reaction\ rate$

$k_{bi} = backward\ reaction\ rate$

ν_{ij}'' and ν_{ij}' = stochiometric coefficients

CIRE Lab

CESE 1D Solver Features

- Solver implements well known a-α numerical scheme
  - To accurately resolve flow discontinuities such a shock waves
- Courant Number insensitive scheme
  - To decrease numerical diffusion at low courant numbers
- Fully-implicit source term implemented
  - Dual time stepping for stiff source terms

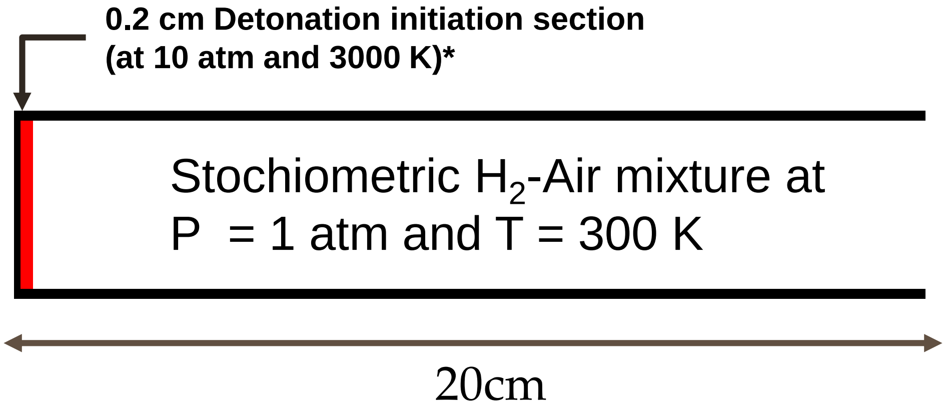
H_2-Air Detonation

- Detonation propagation in H_2/Air mixtures
- Chemical kinetics for a global, 1 step - reversible, Arrhenius-type chemical reaction for four species: H_2, O_2, N_2 and H_2O adopted

$$2H_2 + O_2 \leftrightarrow 2H_2O$$

$$k_f = A_f \exp\left({}^{-T_f}/_{T}\right)$$

$$A_f = 1.102 \times 10^{13}\ {}^{1}/_{sec}, T_f = 8052\ K$$

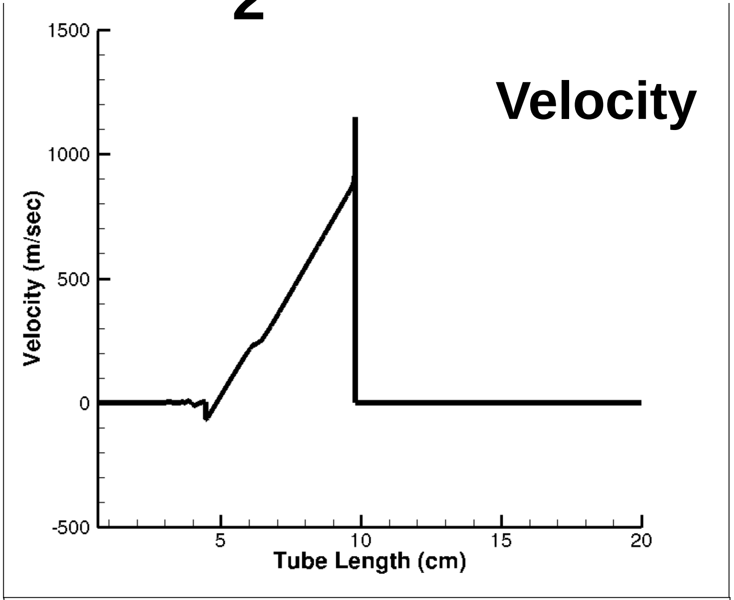


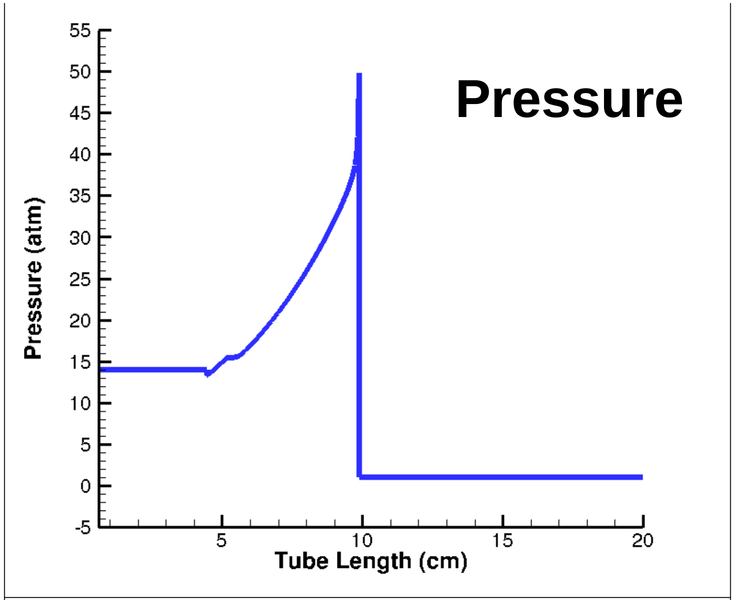
0.2 cm Detonation initiation section (at 10 atm and 3000 K)*

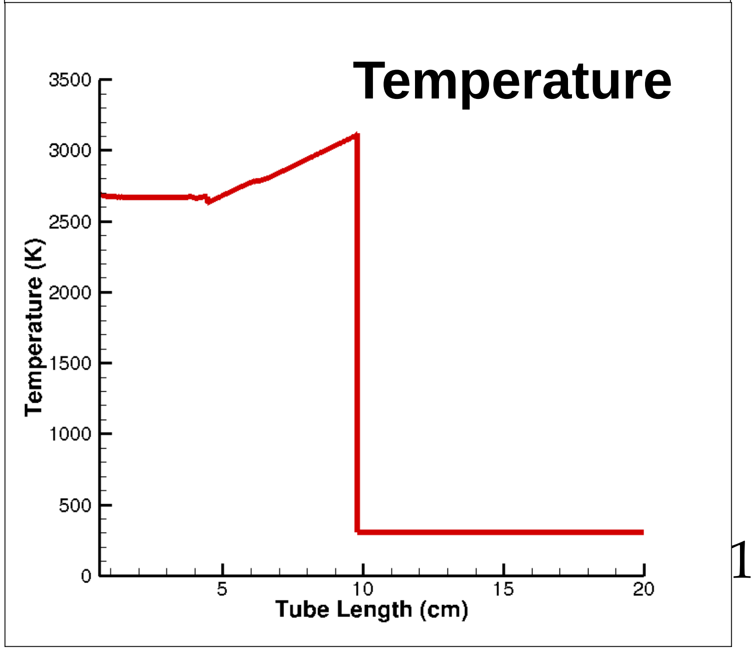
Stochiometric H_2-Air mixture at P = 1 atm and T = 300 K

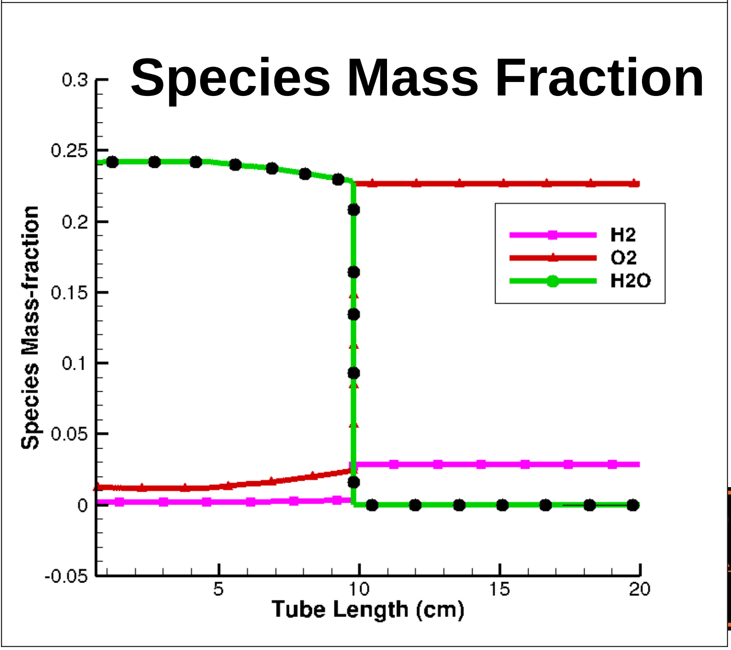
20cm

H_2-Air Detonation Results









Oxy-Fuel Reduced Kinetics

Westbrook-Dryer (WD)

- Widely used for turbulent flame combustion modeling with air
- No dissociation reactions accounted, hence over predicts adiabatic flame temperature

Jones-Lindstedt revised (JL-R)

- Accounts O_2 dissociation; accurate prediction of adiabatic flame temperature

JL-R Mechanism

1) $CH_4 + 0.5\,O_2 \rightarrow CO + 2H_2$

2) $CH_4 + H_2O \rightarrow CO + 3H_2$

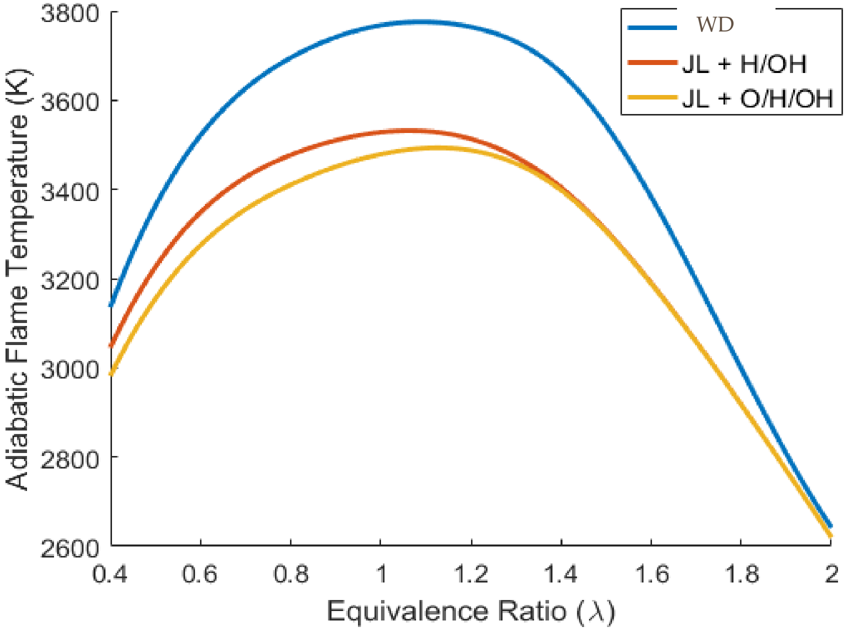
3) $CO + H_2O \leftrightarrow CO_2 + H_2$

4) $H_2 + 0.5\,O_2 \leftrightarrow H_2O$

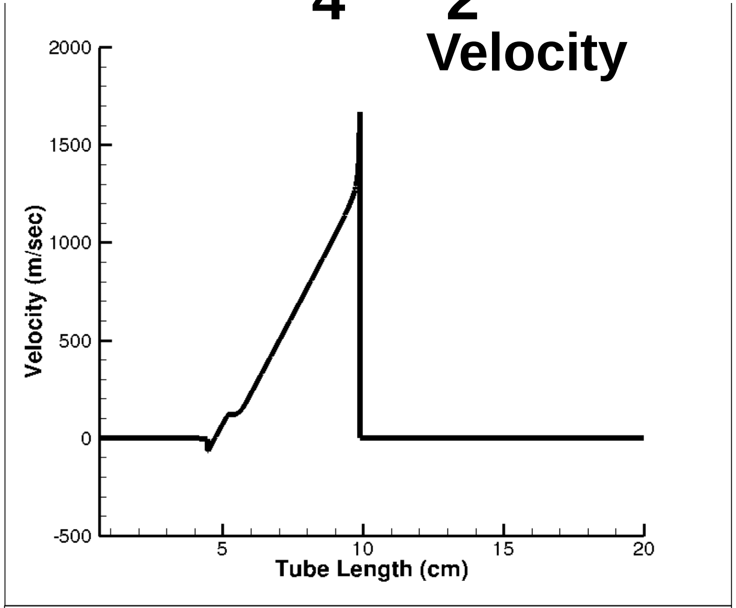
5) $O_2 \leftrightarrow 2O$

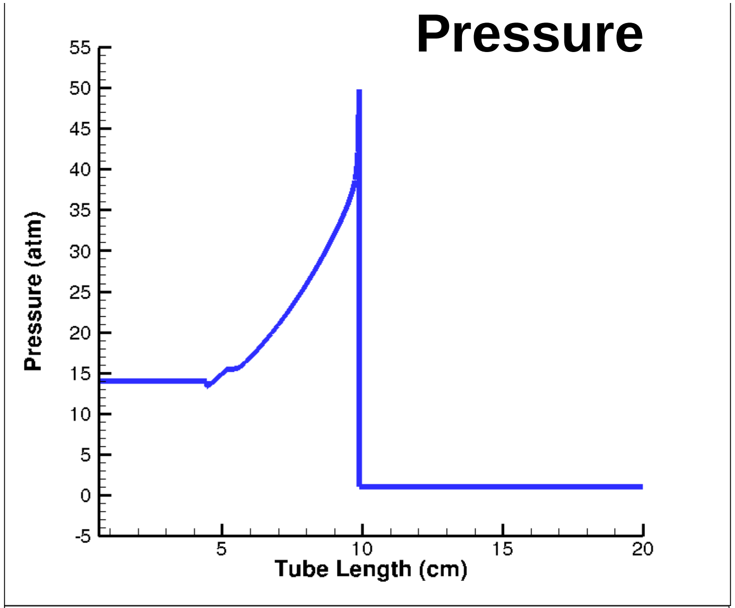
6) $H_2O \leftrightarrow H + OH$

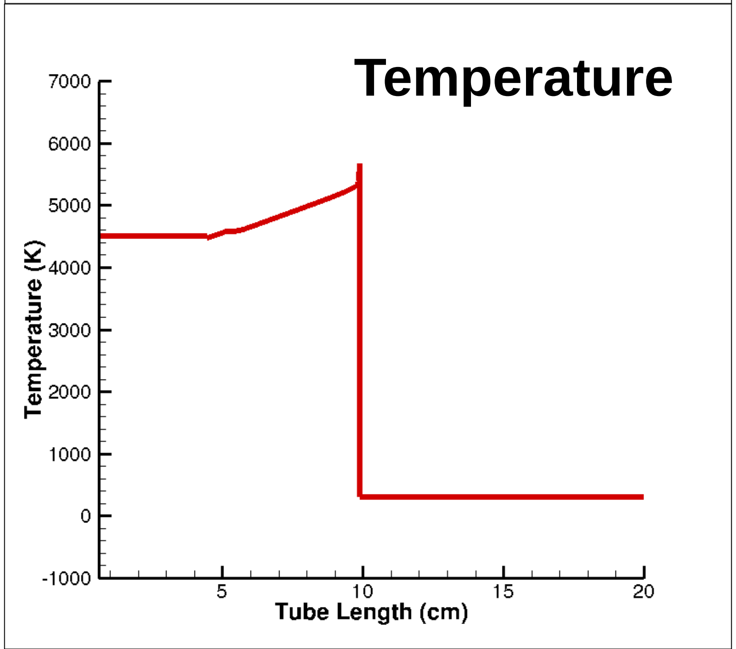
Adiabatic Flame temperature, WD and JLR mechanisms

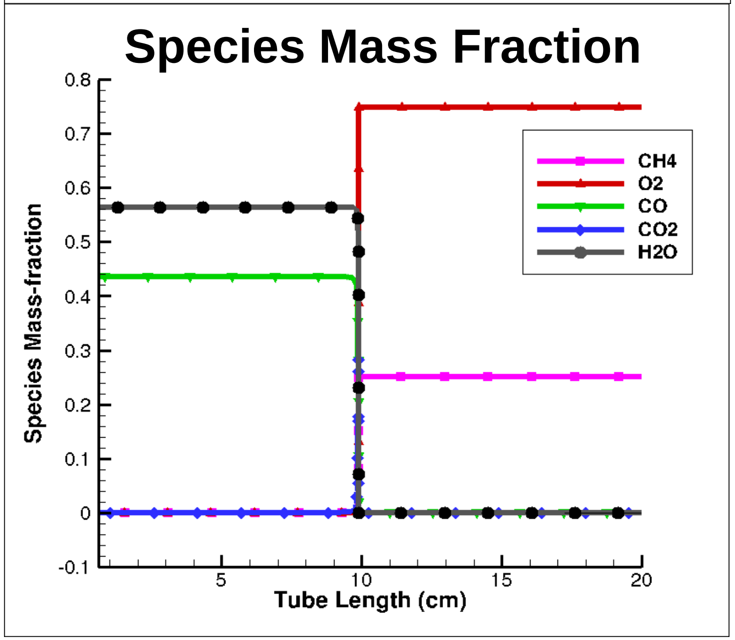


CH_4-O_2 Detonation Results


Velocity


Pressure


Temperature

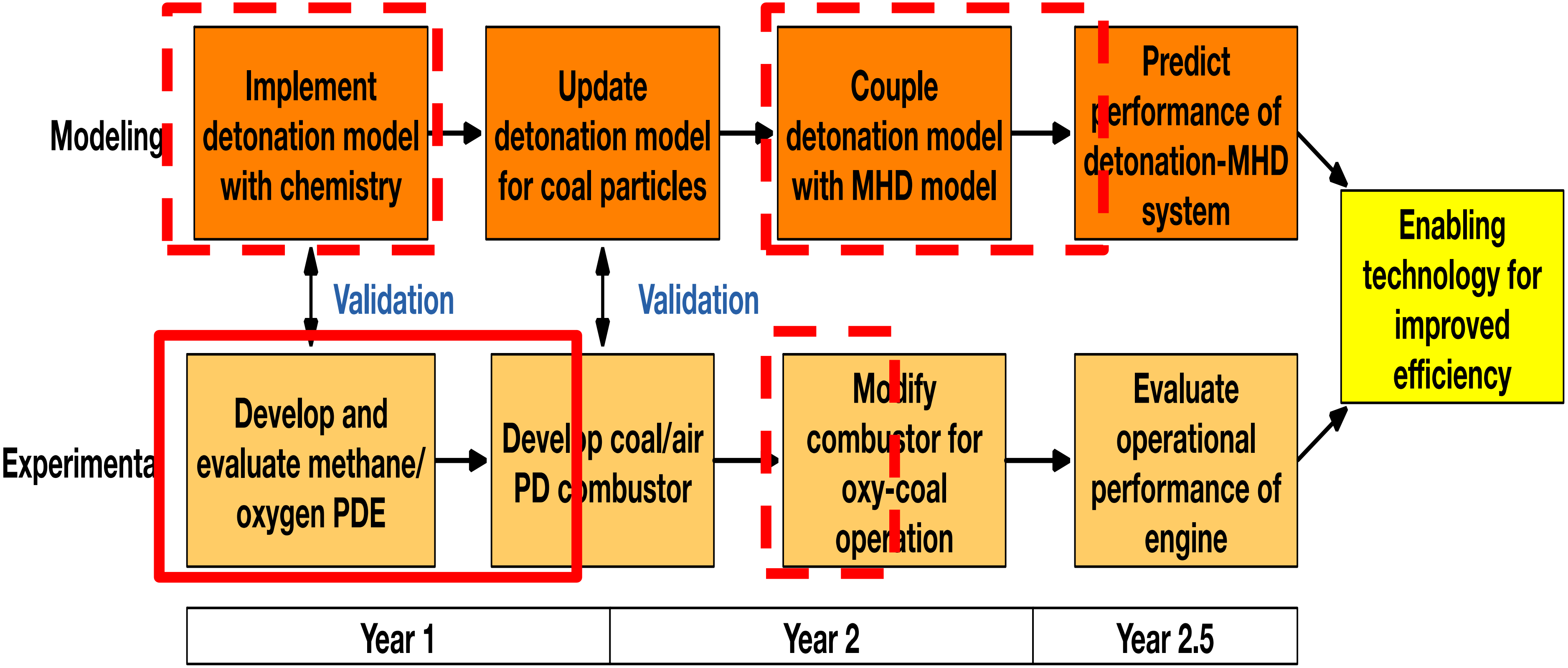

Species Mass Fraction

Use of Coal for Detonations

- Coal abundant resource in United States (and funding specific to its use)
- Prior (limited) research has considered detonations coupled with MHD for gaseous fuels
- Most research investigating coal detonations has focused on safety
- Physical and thermal properties of coal detonations need to be measured to understand coupling with MHD

Anthracite coal, picture courtesy of Wikipedia

Overview of Tasks


Modeling

Implement detonation model with chemistry

Update detonation model for coal particles

Couple detonation model with MHD model

Predict performance of detonation-MHD system

Validation

Validation

Experimental

Develop and evaluate methane/ oxygen PDE

Develop coal/air PD combustor

Modify combustor for oxy-coal operation

Evaluate operational performance of engine

Enabling technology for improved efficiency

Year 1	Year 2	Year 2.5

CIRELab

Future Work

Experimental

1) Transition PDE to operate using oxy-coal
2) Measure boundary conditions and velocities for calculations
3) Quantify changes in detonation characteristics between solid and gaseous fuels

Computational

1) Couple MHD solver with detonation code
2) Develop detonation code
3) Parametric study of MHD performance for detonations (long-term)

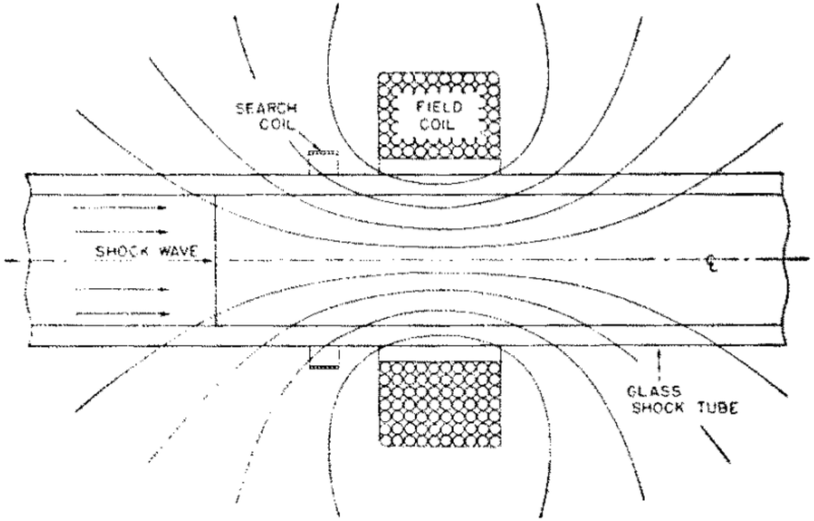
Conductivity analysis

$$\sigma^* = \frac{u_c^2 \sigma_C I_c}{\Phi_c} \psi_2 \frac{\Phi}{U u_2 I}$$ [1]

Calibration values

Assumed conductivity distribution

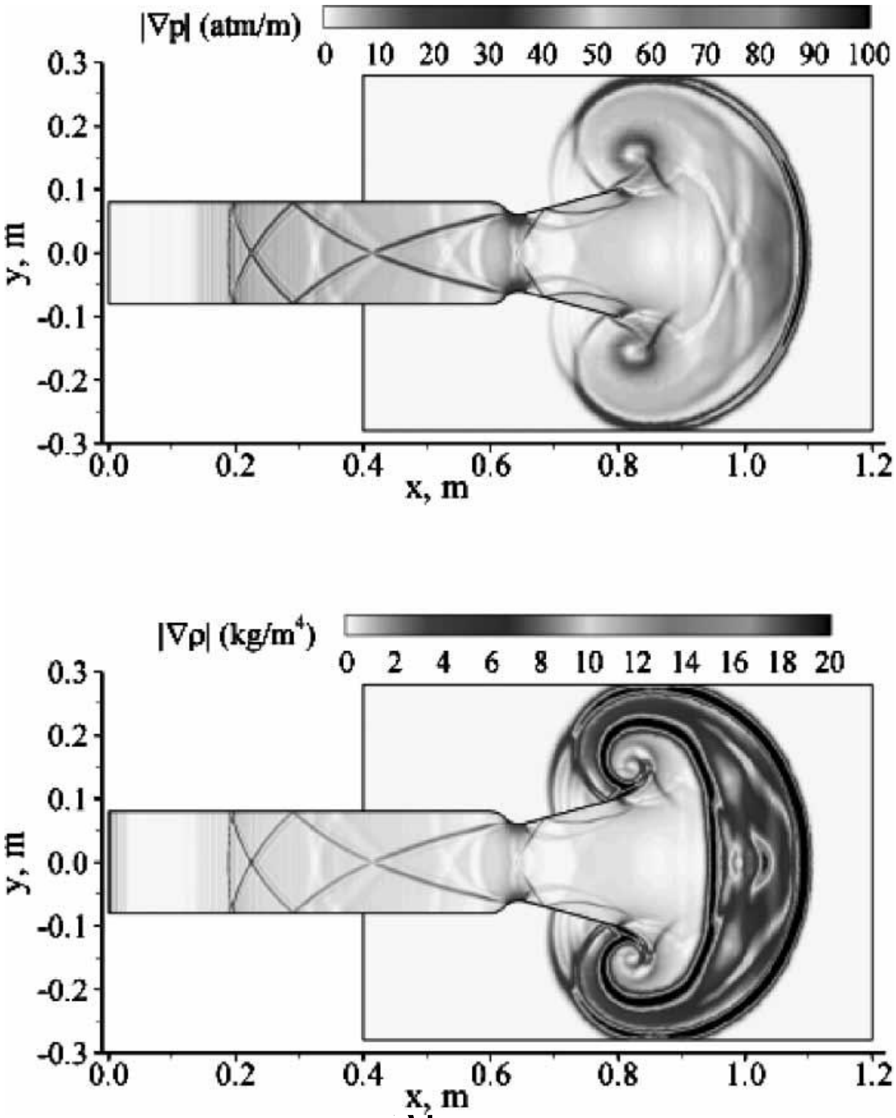
Experimental values



[1]

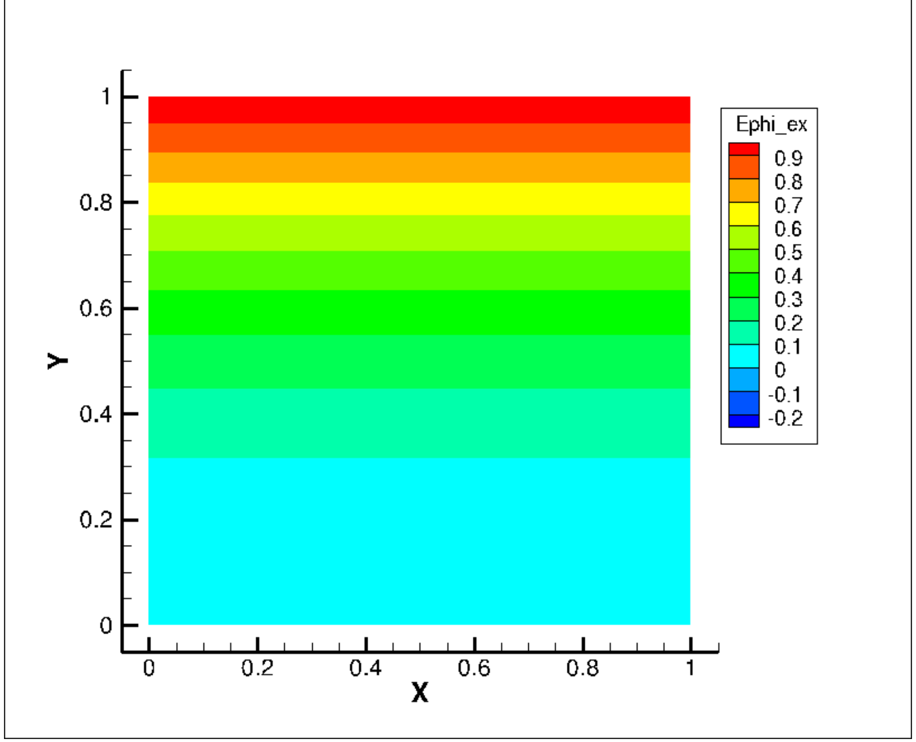
1. Shao Chi Lin, E. L. Resler, and Arthur Kantrowitz. Electrical conductivity of highly ionized argon produced by shock waves. Journal of Applied Physics, 26(1):95–109, 1955.

CE/SE Method: 2D Detonation Example

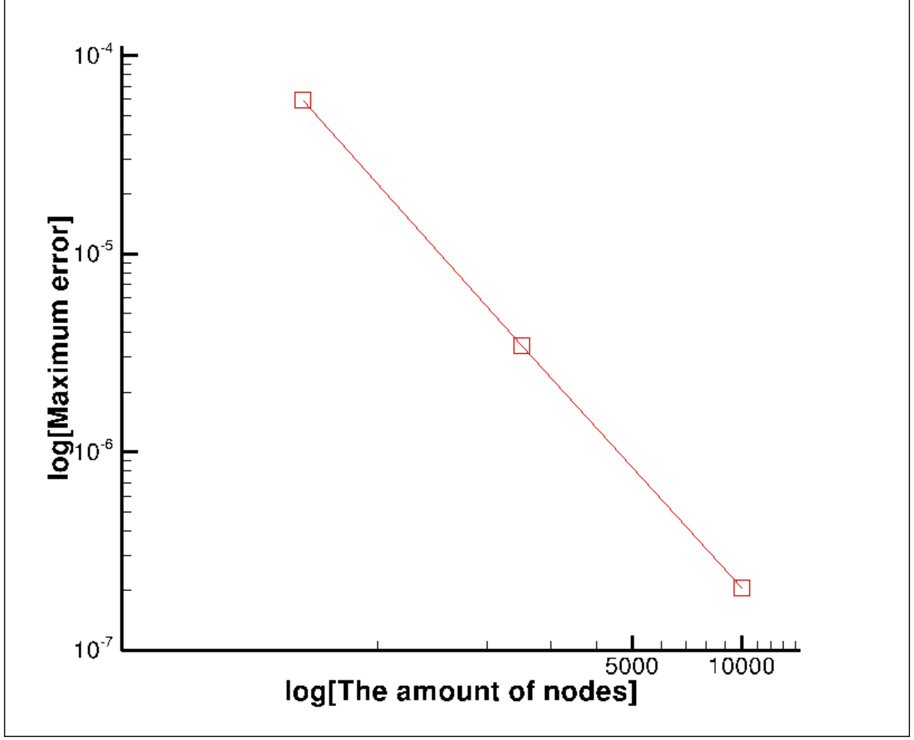


Wu, Ma, and Yang [14]

Test Case for Electric Field



Distribution of electric potential



Maximum error for an amount of node

Conditions

$\sigma = 1\ \mathrm{S/m}$

$\beta = 2$

$|\boldsymbol{B}| = 3\ \mathrm{T}$

$u_x = -\cos 2\pi x \sin 2\pi y$

$u_y = \cos 2\pi y \sin 2\pi x$

No Exact Solution

Manufactured Solution

$\phi =$

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[11] Cambier J-L, Lofftus D. MHD Power Generation From a Pulse Detonation Rocket Engine. 33rd AIAA Plasmadynamics & Lasers Conference, 2002, pp. 49–

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