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

PI: David L. Blunck, Welty Faculty Fellow
Oregon State University
Co-PI: Kyle Niemeyer and Sourabh Apte

Funding from NETL (FE0025822), Oregon BEST, ONR YIP Award (12045202), and NASA Space Grant gratefully acknowledged

PROPULSION LABORATORY

CIRE Lab

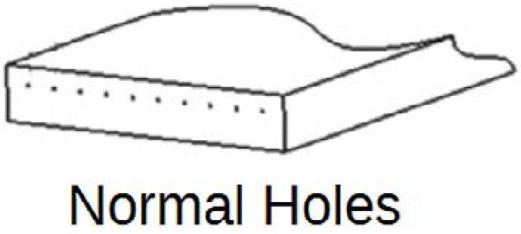
Acknowledgements

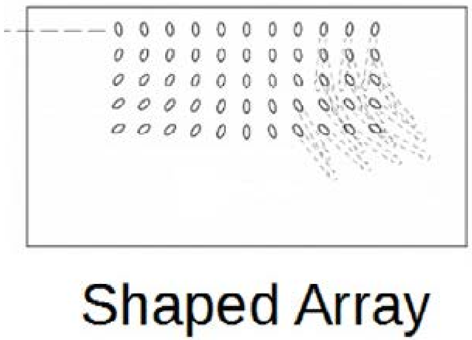
Students: Matthew Zaiger, Derek Bean, Shahank Karra, Rachel Nelke, Peter Beck, Zach Powell, Austin Rose, Matthew Hoeper

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

Motivation

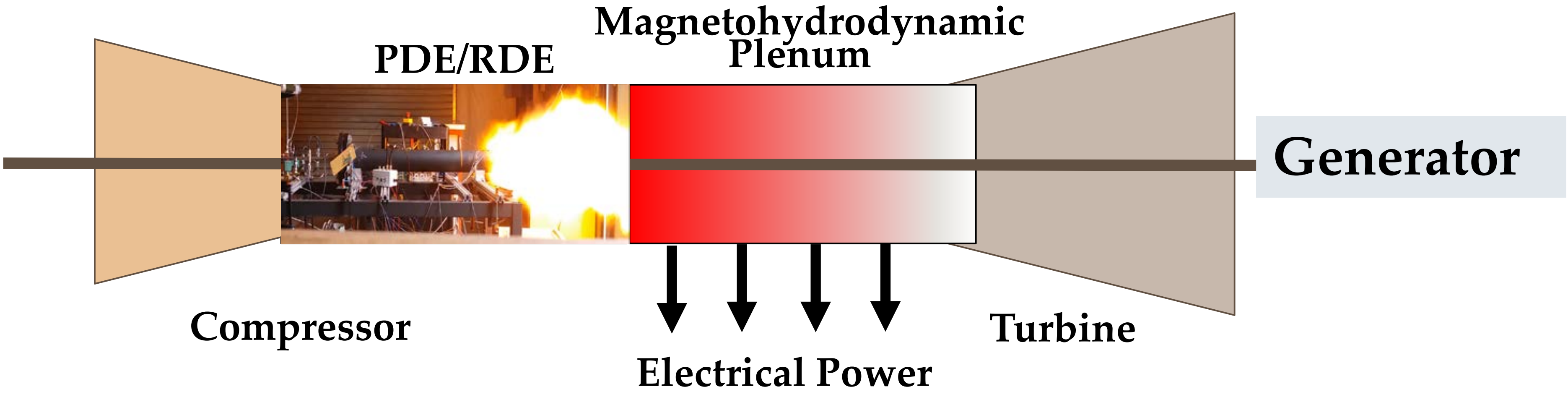
- Improvements in thermodynamic efficiency of power plants needed
- Pressure gain combustion using detonations can significantly improve efficiency
- Yet ..





Richardson, Blunck et al., Combustion and Flame 2016

Motivation



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

Prior Research

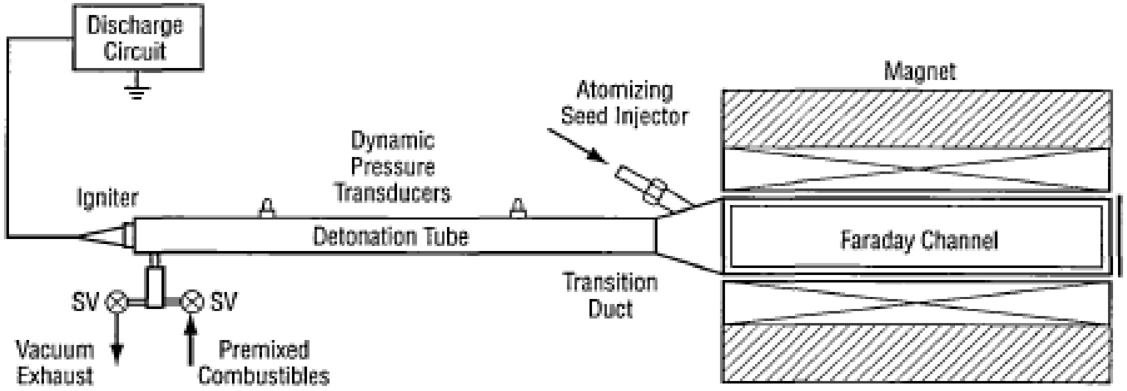


Illustration of detonation and MHD system [Litchford, NASA TP 2001]

Prior research:

- Litchford et al. (NASA) & Cambier et al. (Air Force): MHD power extraction possible from propulsive PDE system
- Matsumoto et al. (2010): hydrogen-air PDE-powered MHD system

Major limitations:

- Primarily propulsive systems; significant insight still needed into interactions between detonation and MHD field
- Coal and CH_4 significantly different than hydrogen

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

Technical Objectives

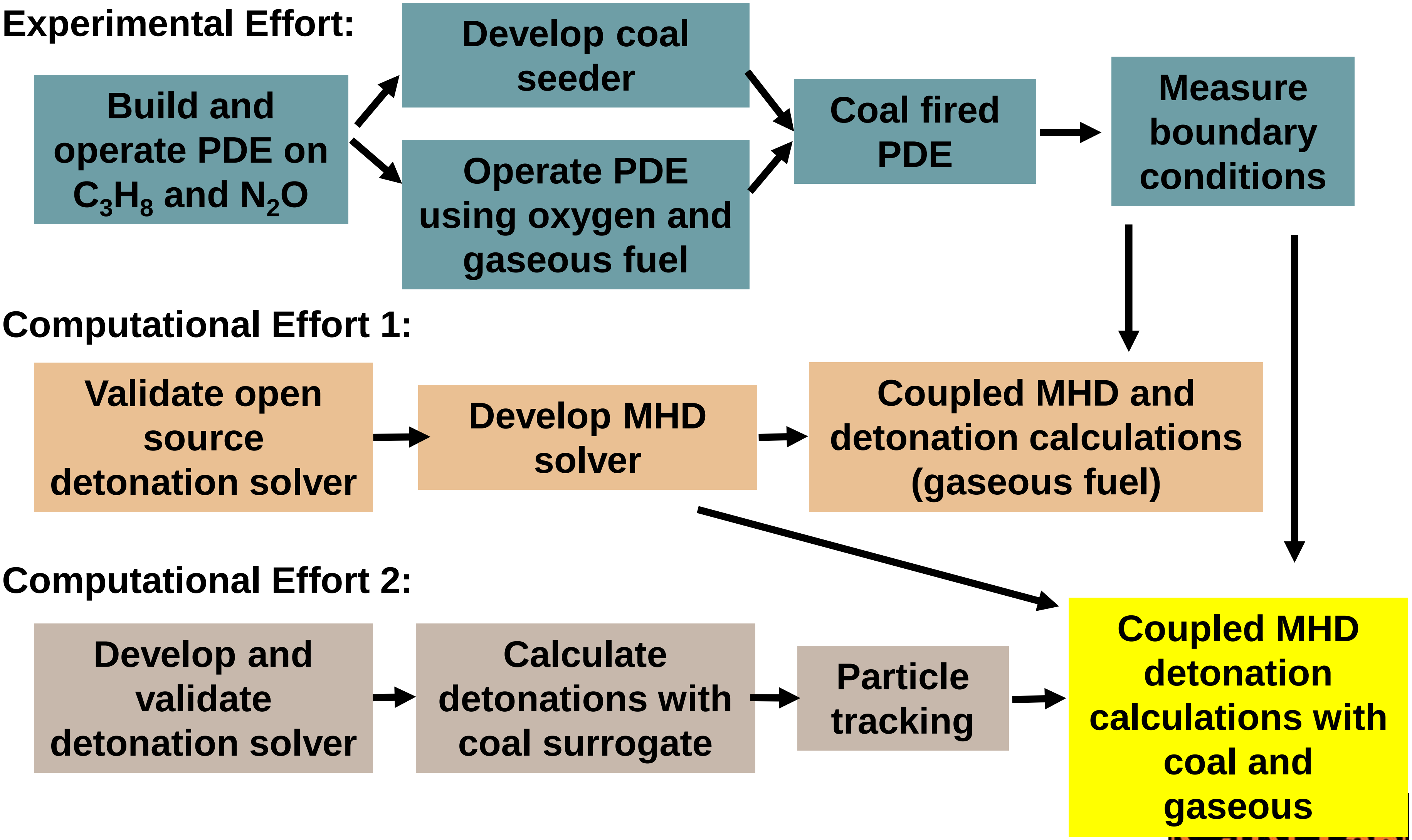
Overall Goal

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:

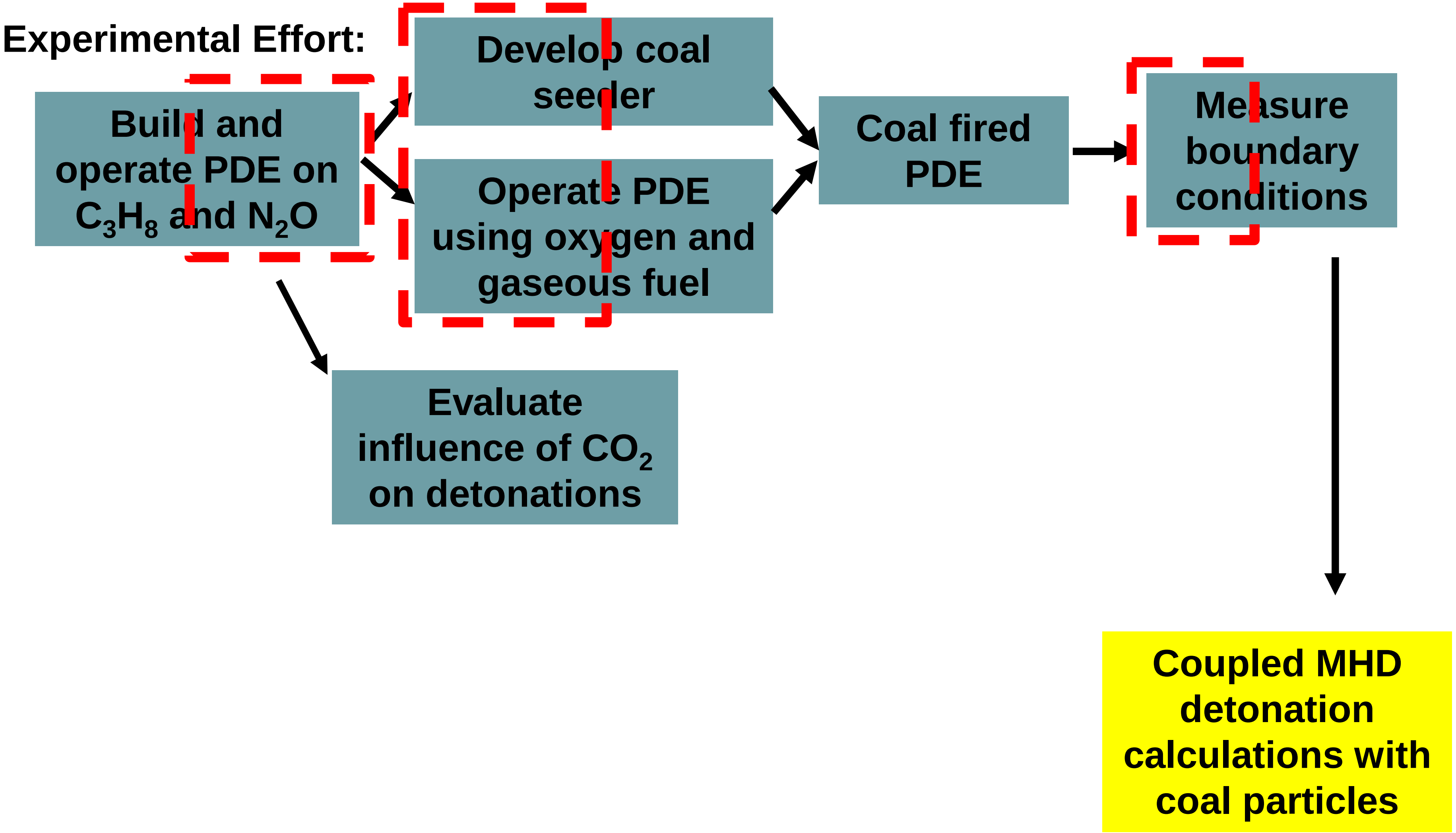
Develop and validate detonation solver

Calculate detonations with coal surrogate

Particle tracking

Coupled MHD detonation calculations with coal and gaseous

Experimental Effort



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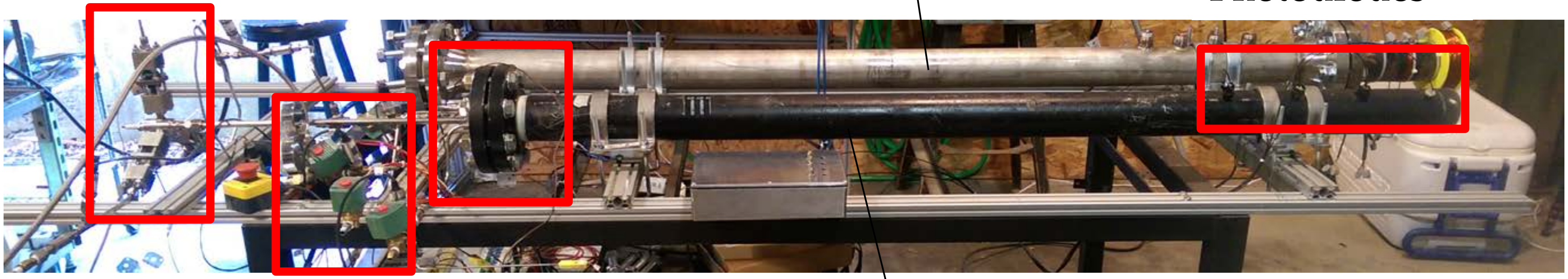
Evaluate influence of CO_2 on detonations

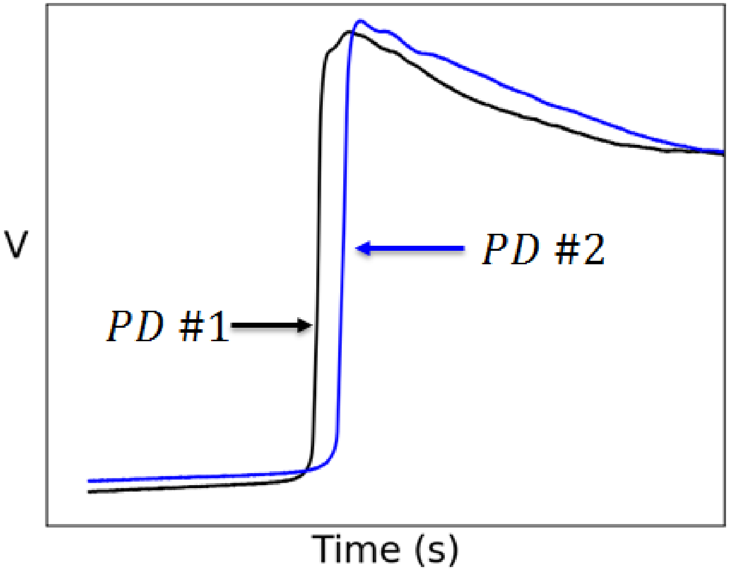
Coupled MHD detonation calculations with coal particles

Pulse Detonation System



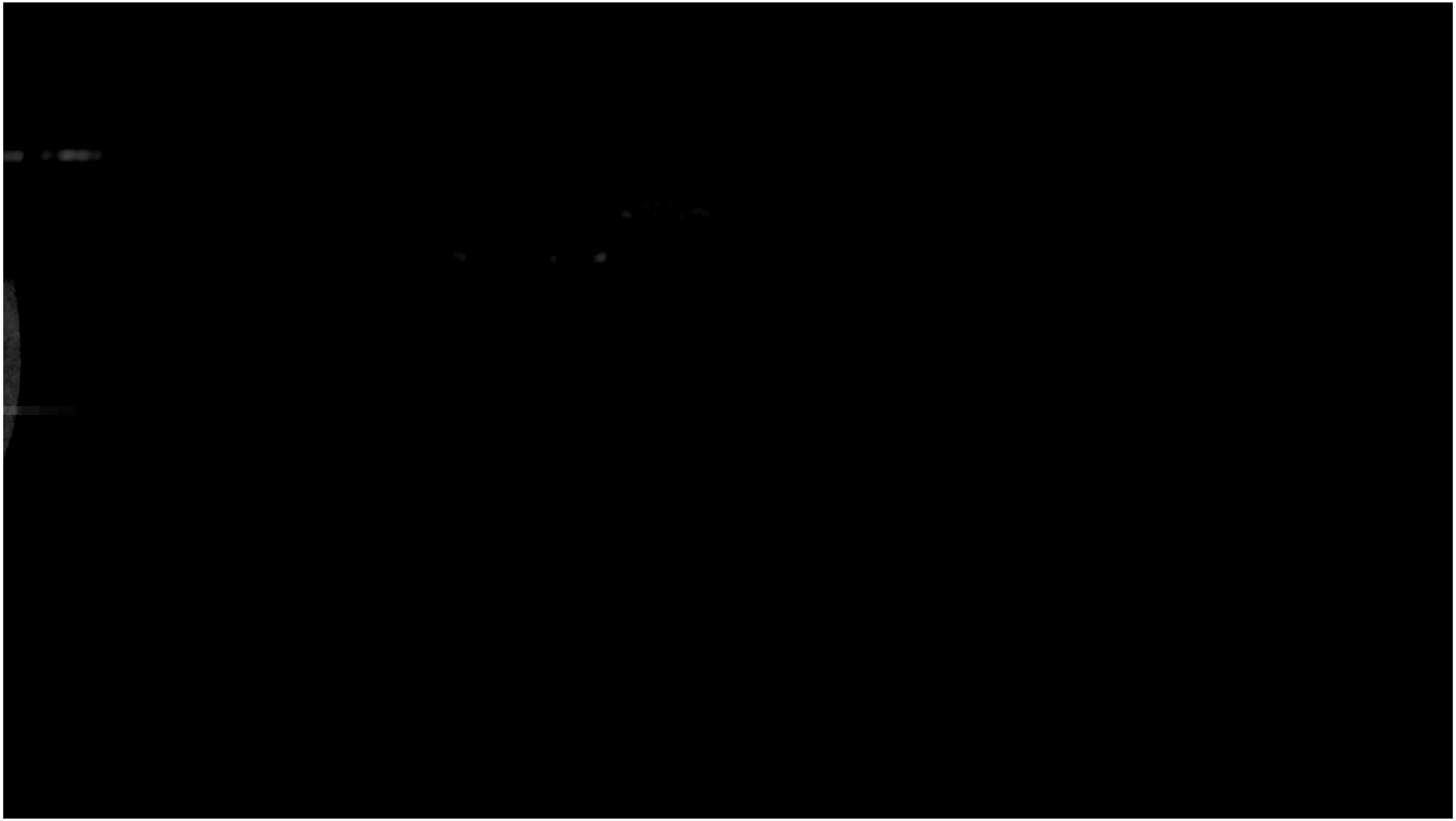
Operating Conditions

- Fuel:C_3H_8
- Oxidizer: N_2O
- Equivalence Ratio: 1
- Frequency: 1~2 Hz (without purge) 0.5 Hz (with purge)
- Detonation velocity: 1920 m/s ± 5% (Averaged over 450+ data sets)
- Estimated error from photodiodes ± 16 m/s



Photodiode voltage response to detonation

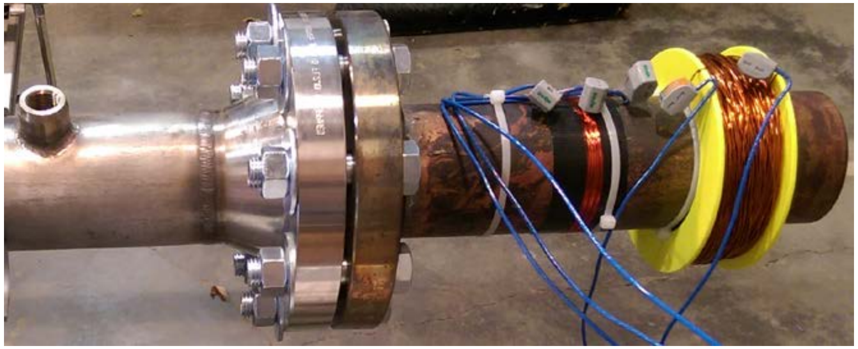
Operation of the PDE

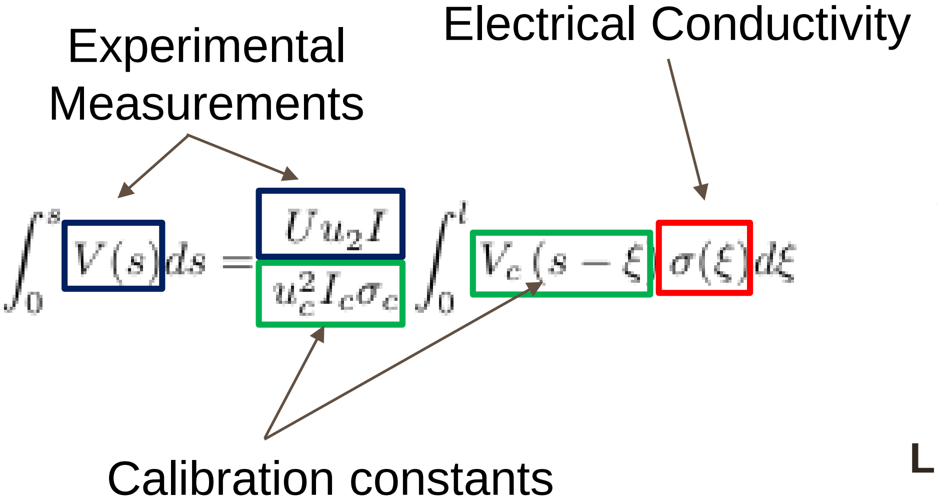


Visible emissions of exhaust from PDE.
Images collected at 8300 fps.

Initial Conditions: Electrical Conductivity

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



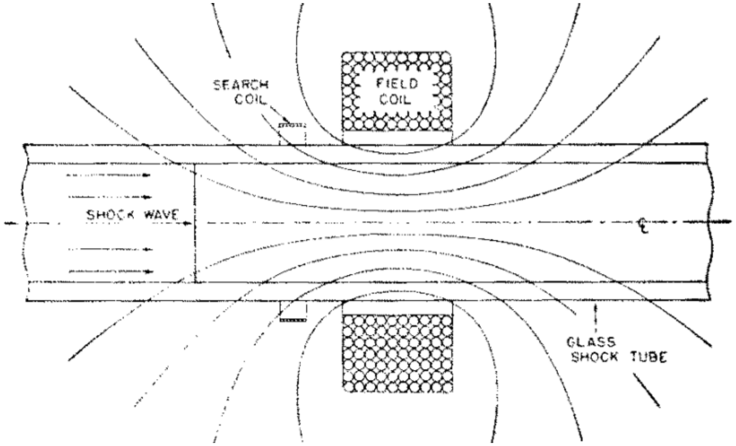


Experimental Measurements

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

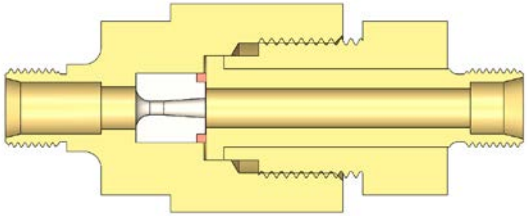


Lin et al., Journal of Applied Physics

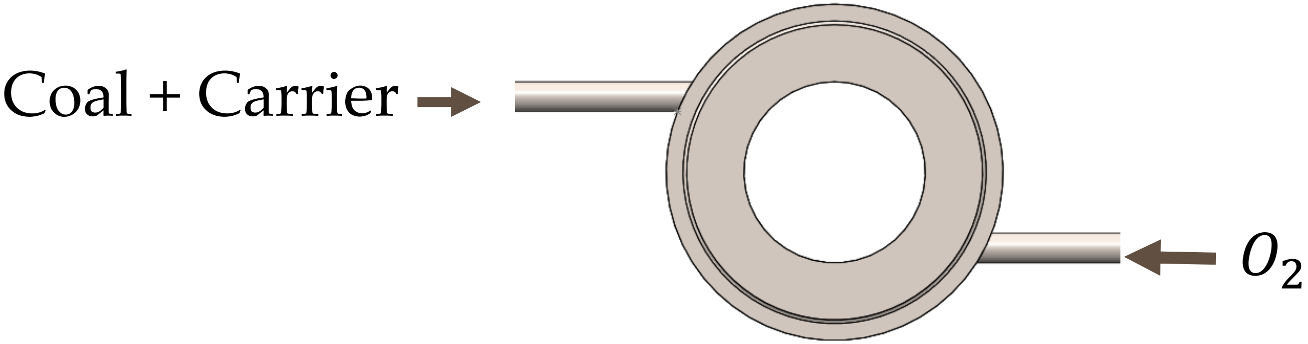
Coal Seeder

Oxygen System

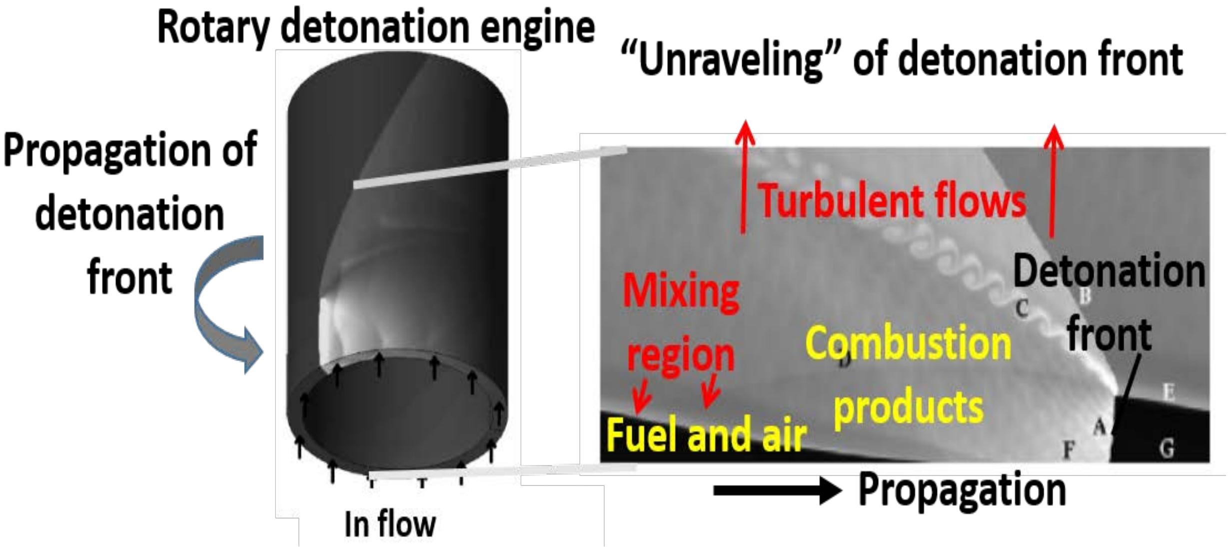
- Oxygen system nearly complete
- Tangential injection of coal and oxygen
    - Minimize impingement velocity
    - Enhance mixing
- Nitrogen purge of O_2 line
- Flow path of O_2 closed on both ends to eliminate particulates and contamination



O_2 injection plumbing



Dilution Effects on Detonation Velocities



Modified from Schwer et al., Proc Comb. Inst. 2011

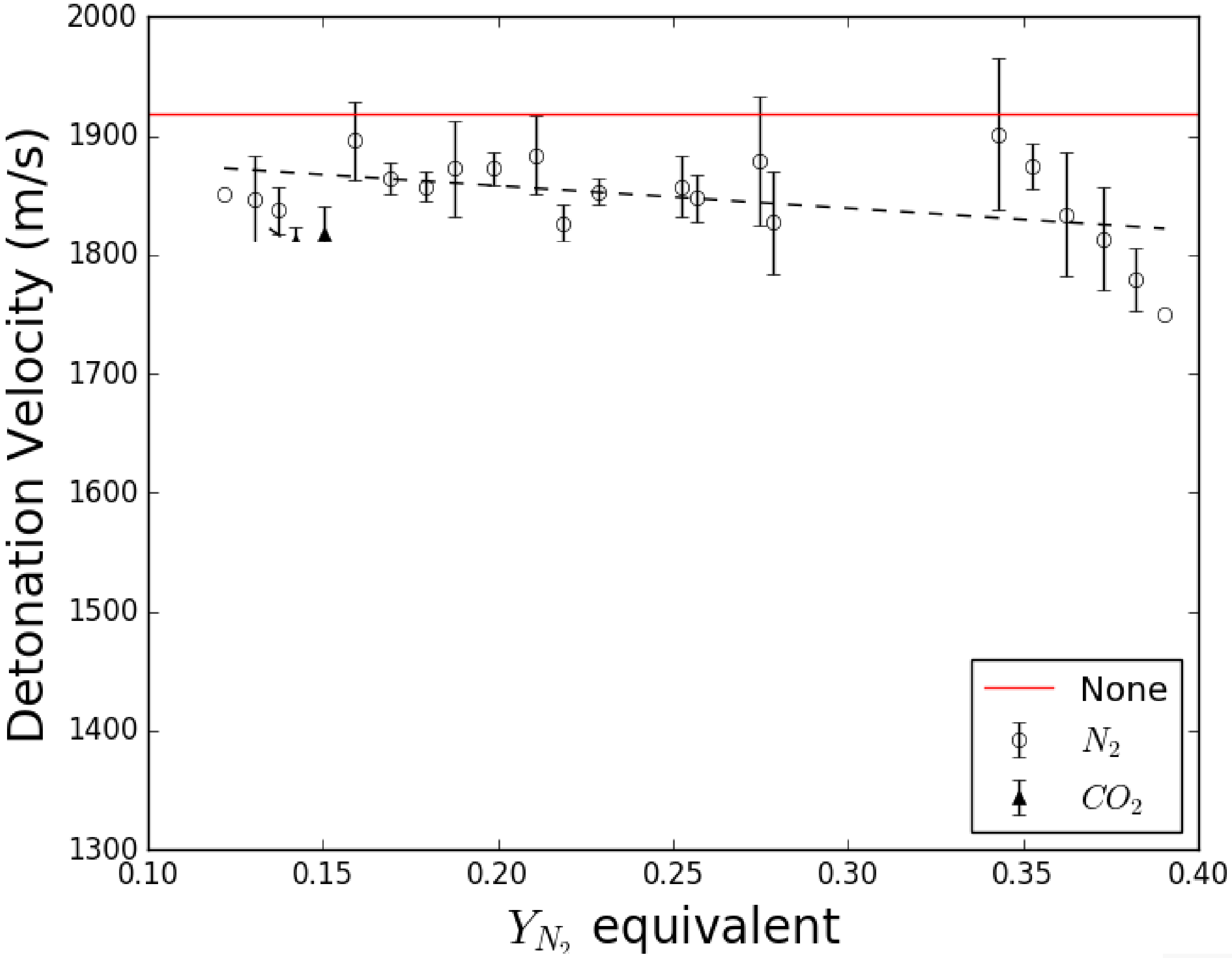
Objective

Identify chemistry and dilution effects of CO_2 on detonation characteristics

Approach

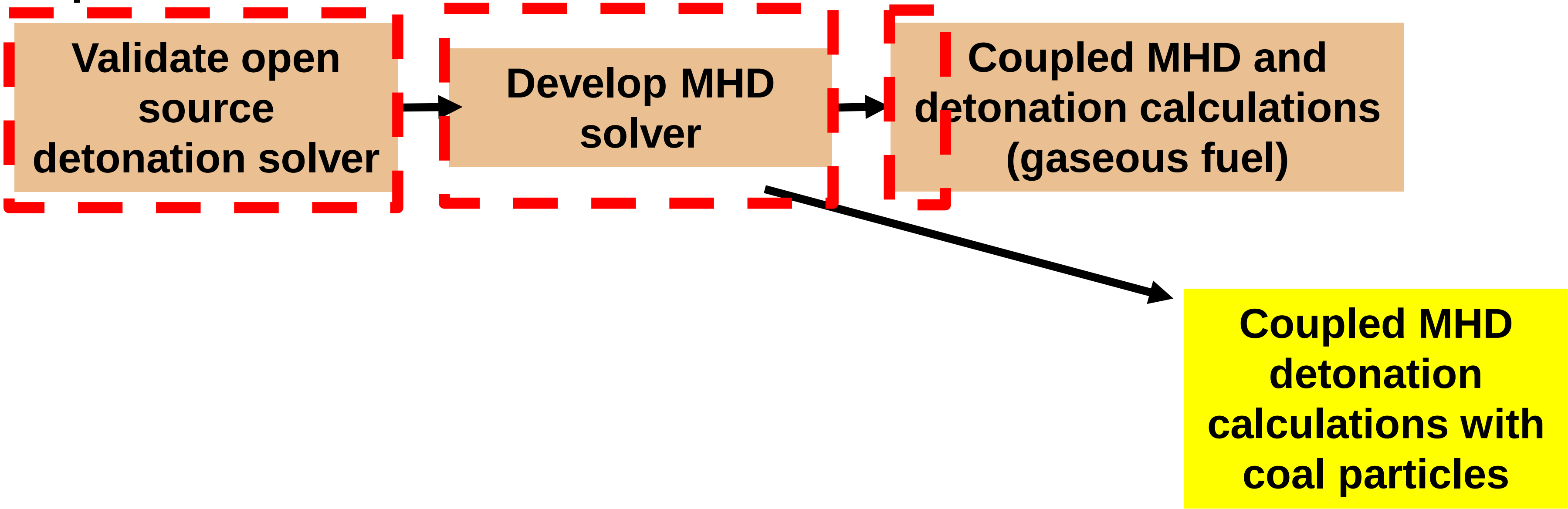
Operate PDE with dilution using N_2 and CO_2

Dilution Effects on Detonation Velocities



Progression of Research

Computational Effort 1:



Validate open source detonation solver

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Coupled MHD and detonation calculations (gaseous fuel)

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

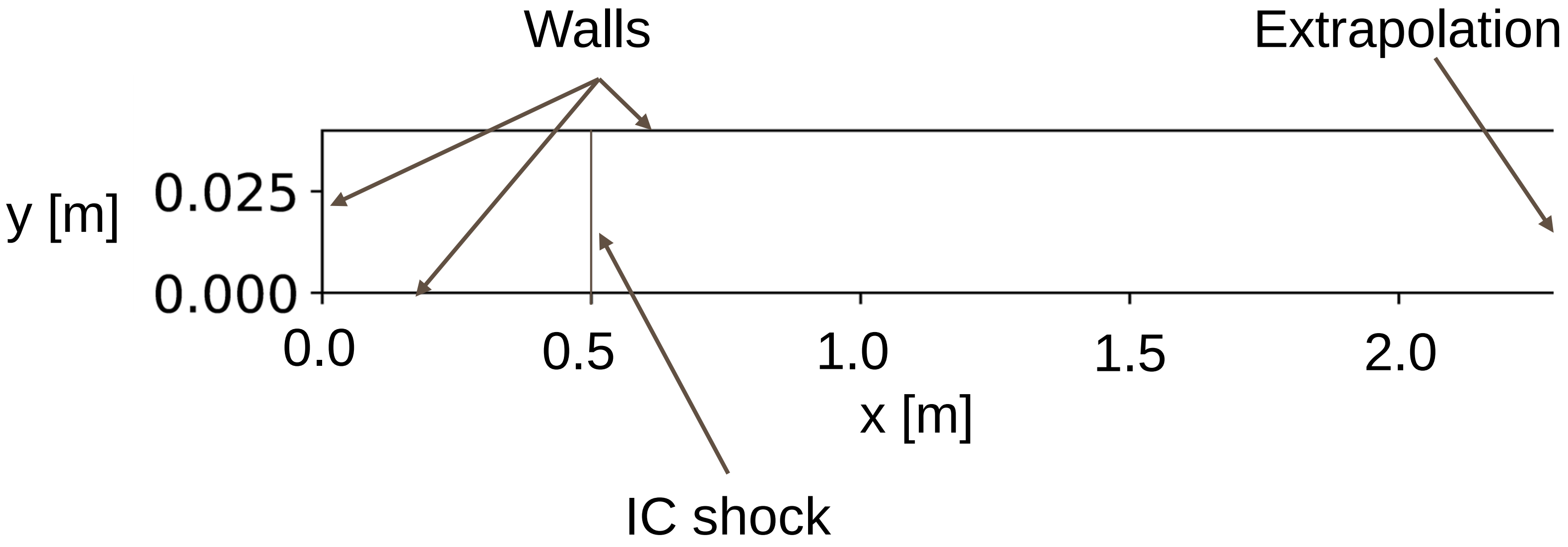
- Kinetics handled by Cantera 2.3.0

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

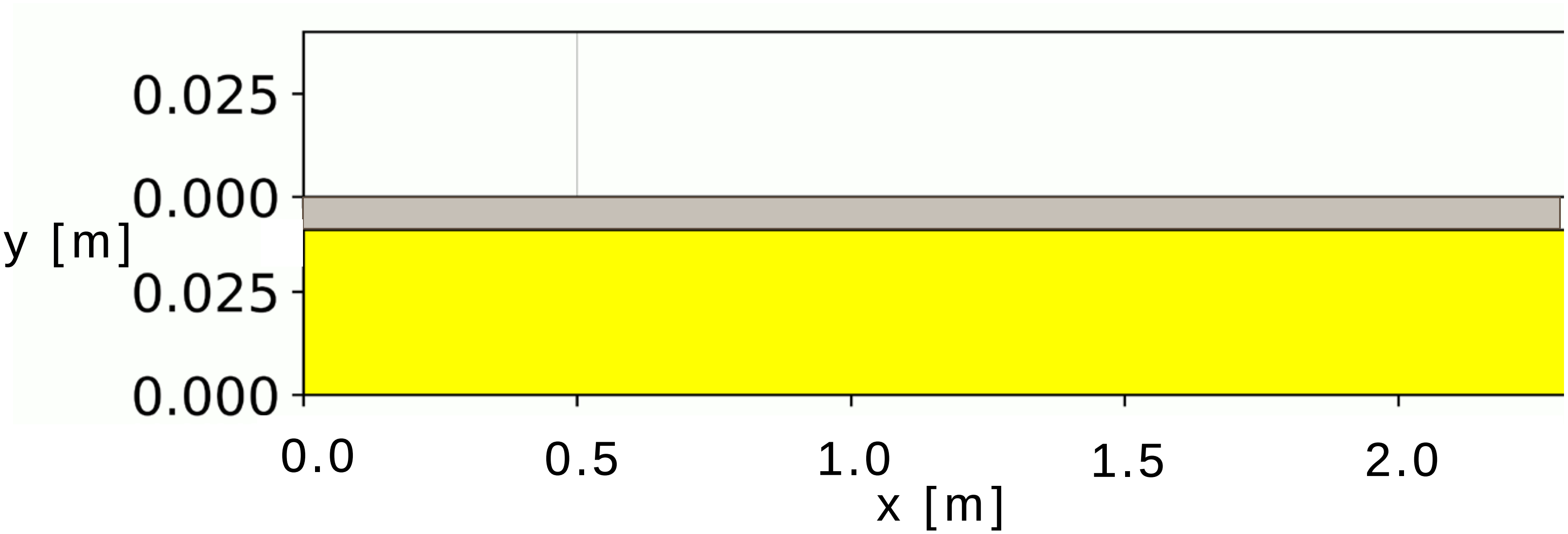
Cantera DOI:10.5281/zenodo.170284,URL: http://www.cantera.org

Operation of the PDE

- Grid resolution – ΔX,Y = 0.0005 [m]
- Initial conditions– standard temperature and pressure
- Boundary conditions – as shown



Operation of the PDE

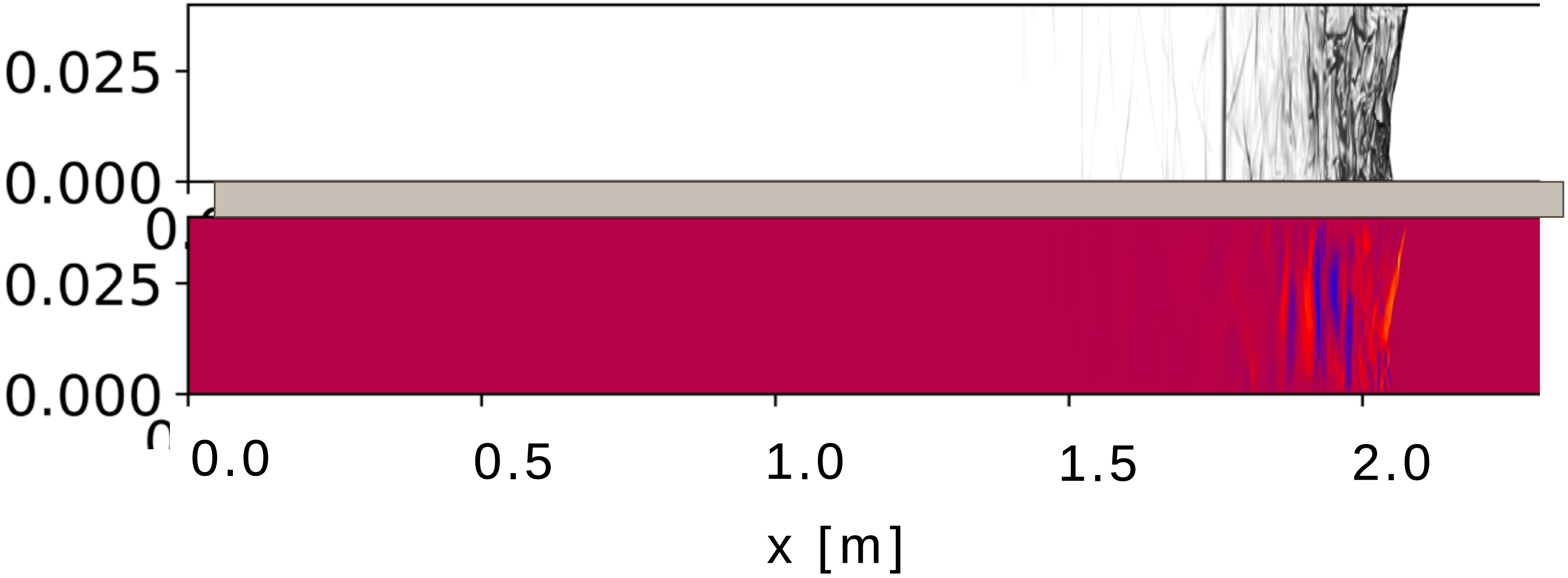


Operation of the PDE

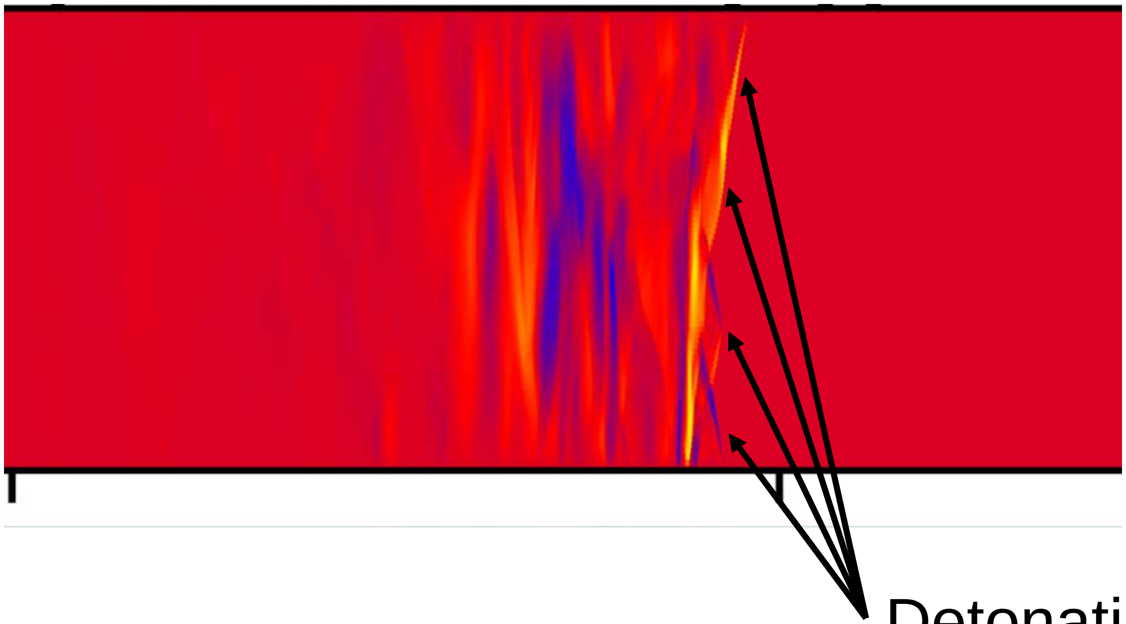
H_2 - O_2 Detonation

Simulation velocity – 2872 [m/s]

Shock & detonation toolbox - 2876 [m/s]

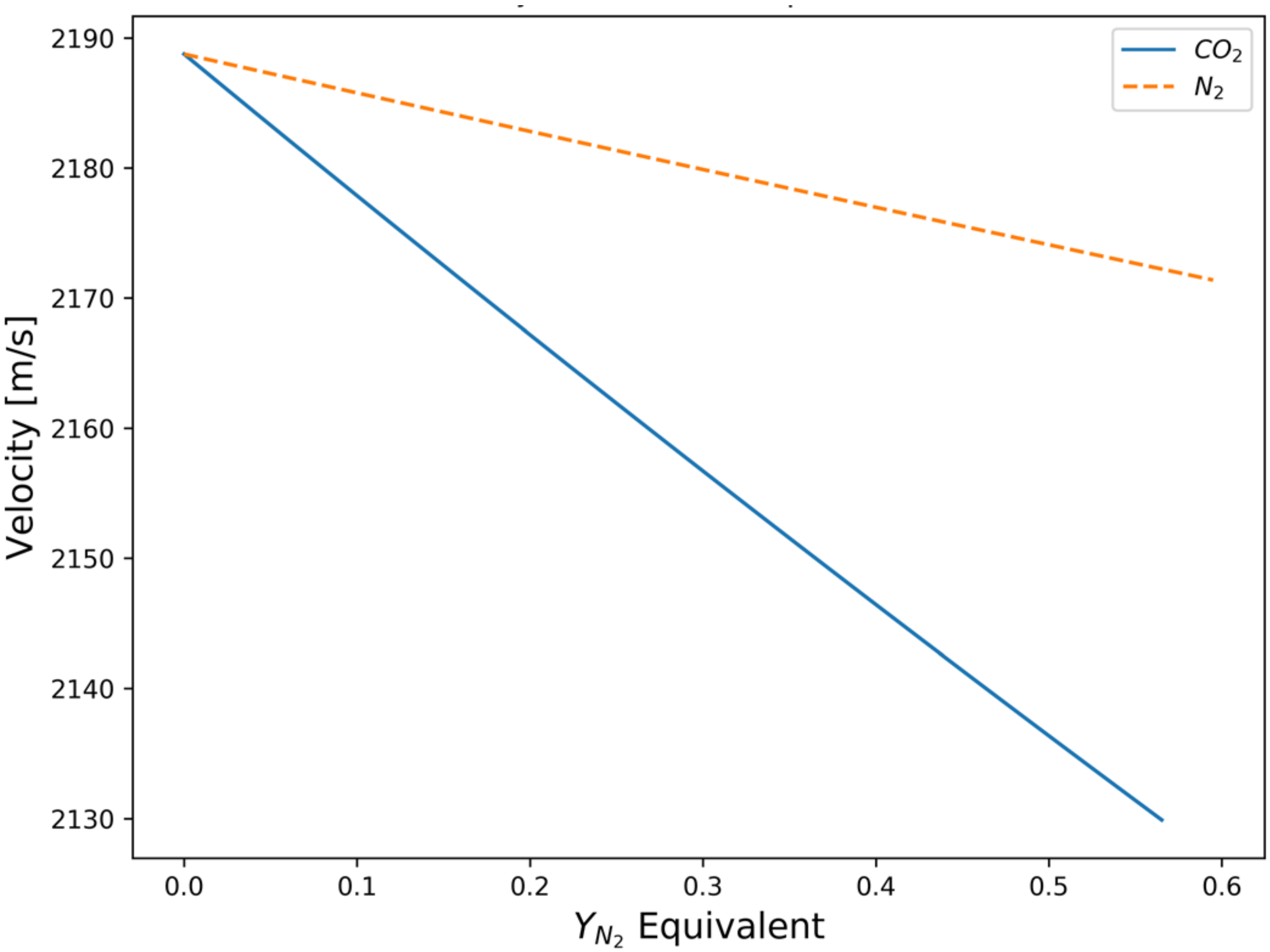


Operation of the PDE



Detonation cells

Dilution Effects on Detonation Velocities: CJ Velocity



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,

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

h: Specific Enthalpy

Y_s: Mass Concentration

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

c_p: Specific Heat at Constant Pressure

Mass conservation equation of Chemical Species:

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

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

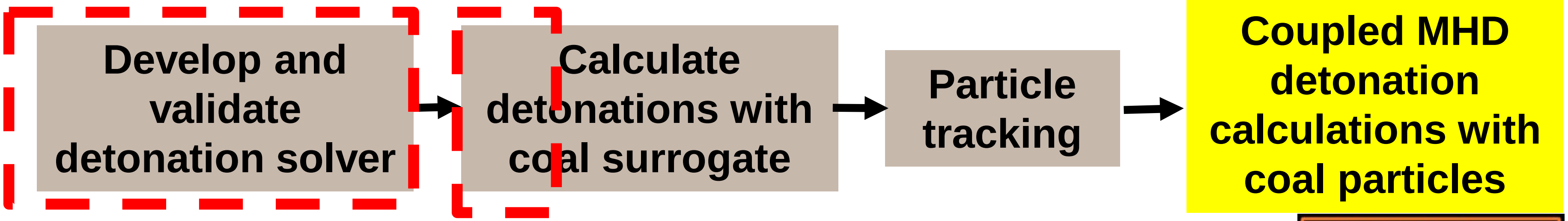
c_e: Electron Mean Thermal Speed

Coupled Detonation and MHD Simulations

- Detonations simulations ready to be performed for C_3H_8 and N_2O
- MHD solver complete
- MHD and detonation simulations started

Progression of Research

Computational Effort 2:



Develop and validate detonation solver

Calculate detonations with coal surrogate

Particle tracking

Coupled MHD detonation calculations with coal particles

Governing Equations for 1D Reacting Flows

Conservation equations for chemically reacting system involving N_s species

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

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

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

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

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

$\rho = density$

$u = velocity$

$C_i = species\ mass\ concentration$

$p = pressure$

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

$species\ per\ unit\ volume$

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

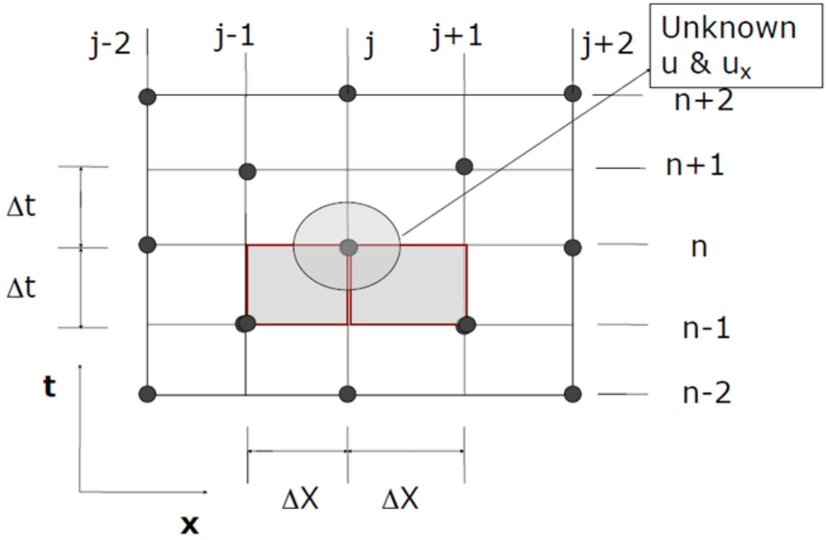
$k_{fi} = forward\ reaction\ rate$

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

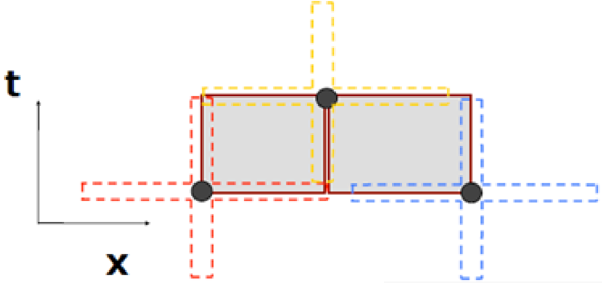
ν_{ij}'' and ν_{ij}' = stochiometric coefficients

Conservation Element (CE) Solution Element (SE) 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)
  - No cell interface Riemann solution needed
- Genuine multi-dimensional formulation
- No dimensional/directional splitting necessary
- Non-dissipative baseline a-scheme
  - Numerical dissipation added as necessary



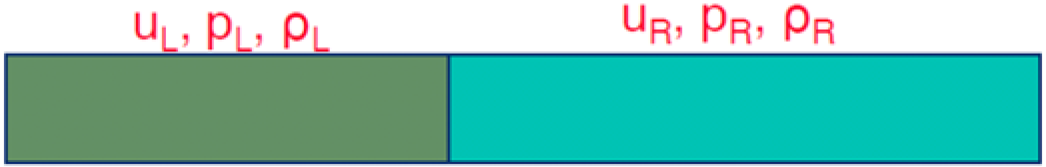
1D CESE Space-Time Staggered Grid*



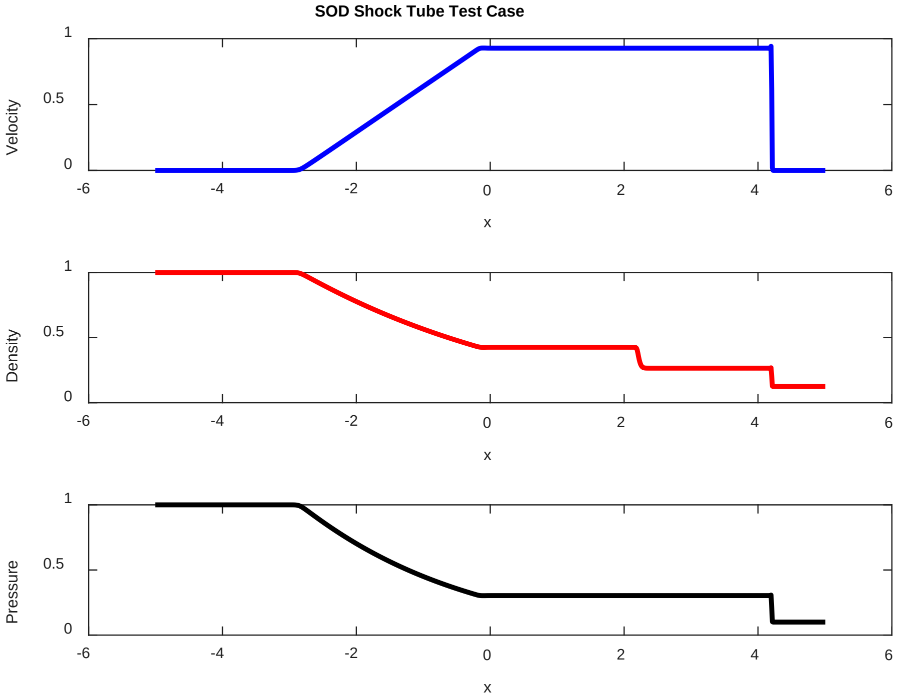
CE (non-overlapping rectangular regions) & SE (dotted lines) *

CESE Solver Validation

- Non-reacting flow case: SOD Shock Tube Case Study



- CESE solver was validated with the classic SOD shock tube problem
- Initial conditions in the tube
  - $(u_l, \quad p_l, \quad \rho_l) = (0, \quad 1, \quad 1)$
  - $(u_r, \quad p_r, \quad \rho_r) = (0, \quad 0.1, \quad 0.125)$

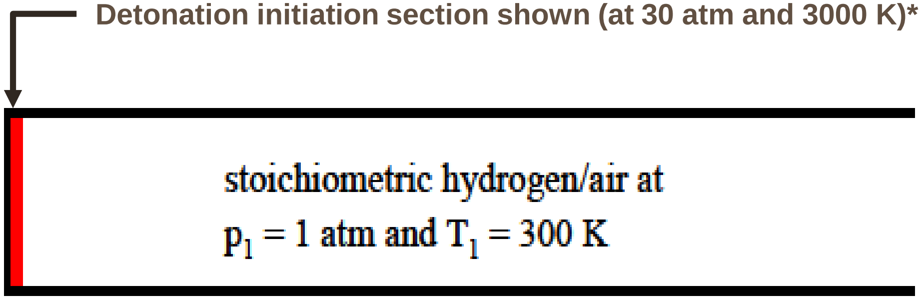


CESE Solver Validation

- Reacting flow case: ZND detonation propagation in a tube
- Arrhenius-type chemical reaction for two species (reactant & product)

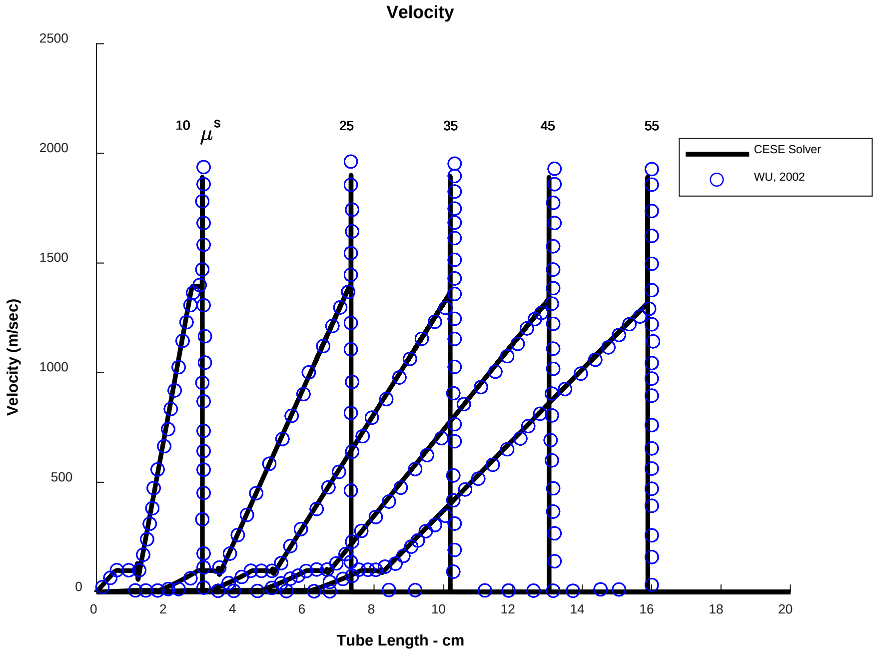
$$Reactant(R) \rightarrow Product(P) + heat\ release(q)$$

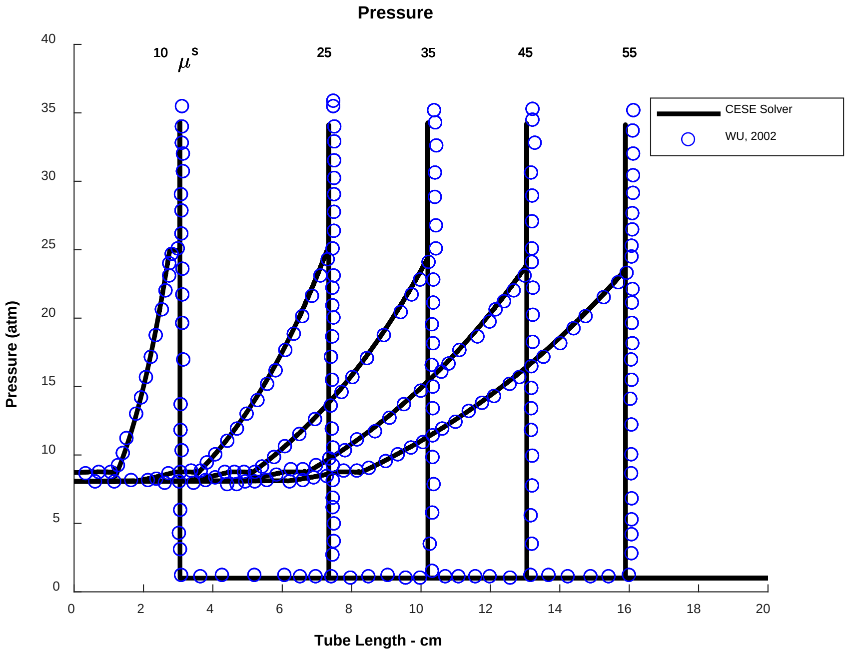
- 20 cm tube filled with premixed stochiometric H_2/O_2 reactant mixture
- 0.2 cm spark region placed near closed head end to initiate detonation
- Results were validated with ZND theory and with Wu, 2002



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

CESE Solver Validation





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

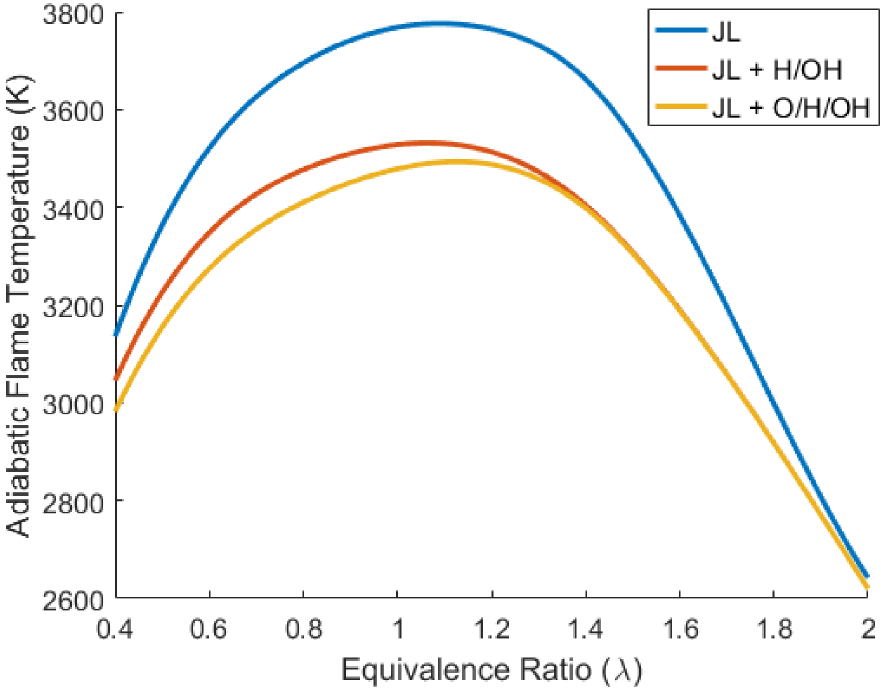
$P_s = \mathit{Von\ Neumann\ pressure\ spike}$

$P_2, T_2 = \mathit{CJ\ pressure}$ and temperature

$P_3 = \mathit{Head\ end\ pressure}$

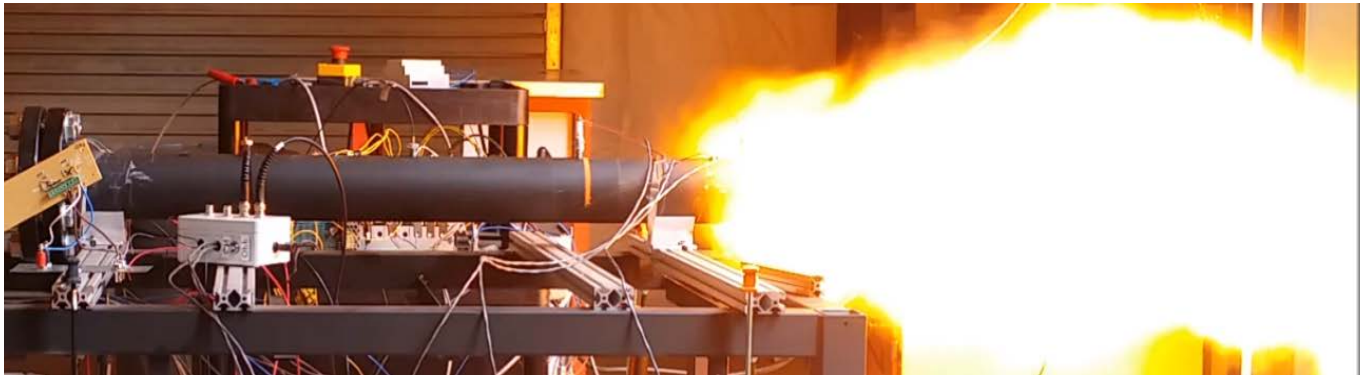
Reduced Reaction Mechanisms for Oxy-Fuel Combustion

- Three reduced reaction mechanisms namely, Westbrook-Dryer (WD), Jones-Lendsedt (JL) & Jones-Lendsedt revised (JL-R), for oxy-methane combustion were implemented and evaluated [Frassoldati et al (2009)]
- JL-R mechanism accounts for dissociation reactions and hence more accurately predicts adiabatic flame temperature for $CH_4 – O_2$ reaction

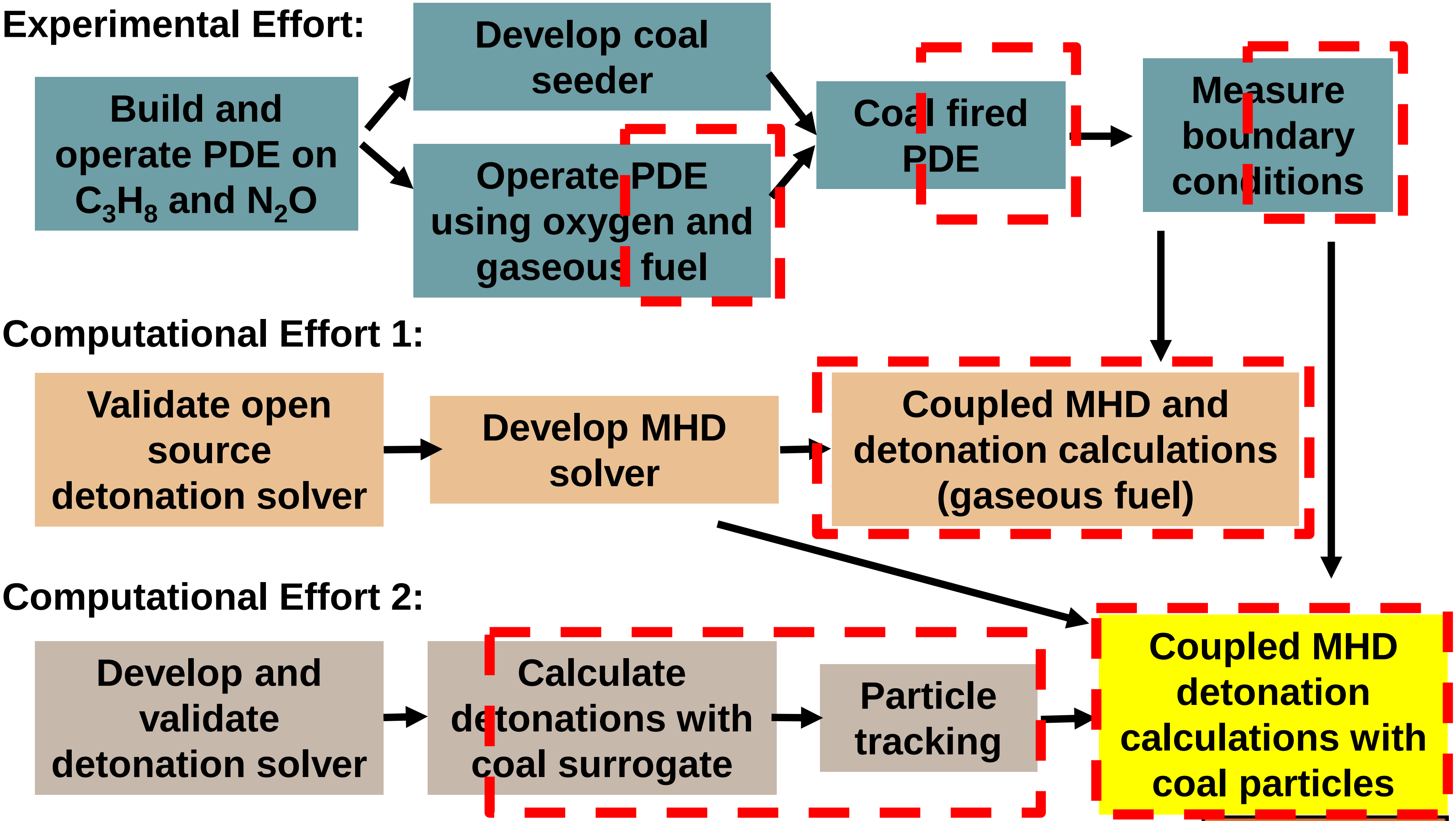


Summary

1) Pulse detonation engine has been developed and applied to study influence of dilution by CO_2
2) Capabilities developed for coal seeding, operation of engine using oxygen, and measuring electrical conductivity
3) Coupled detonation and MHD solver developed
4) In-house detonation solver developed and surrogate for oxy-fuel combustion prepared



Future Work



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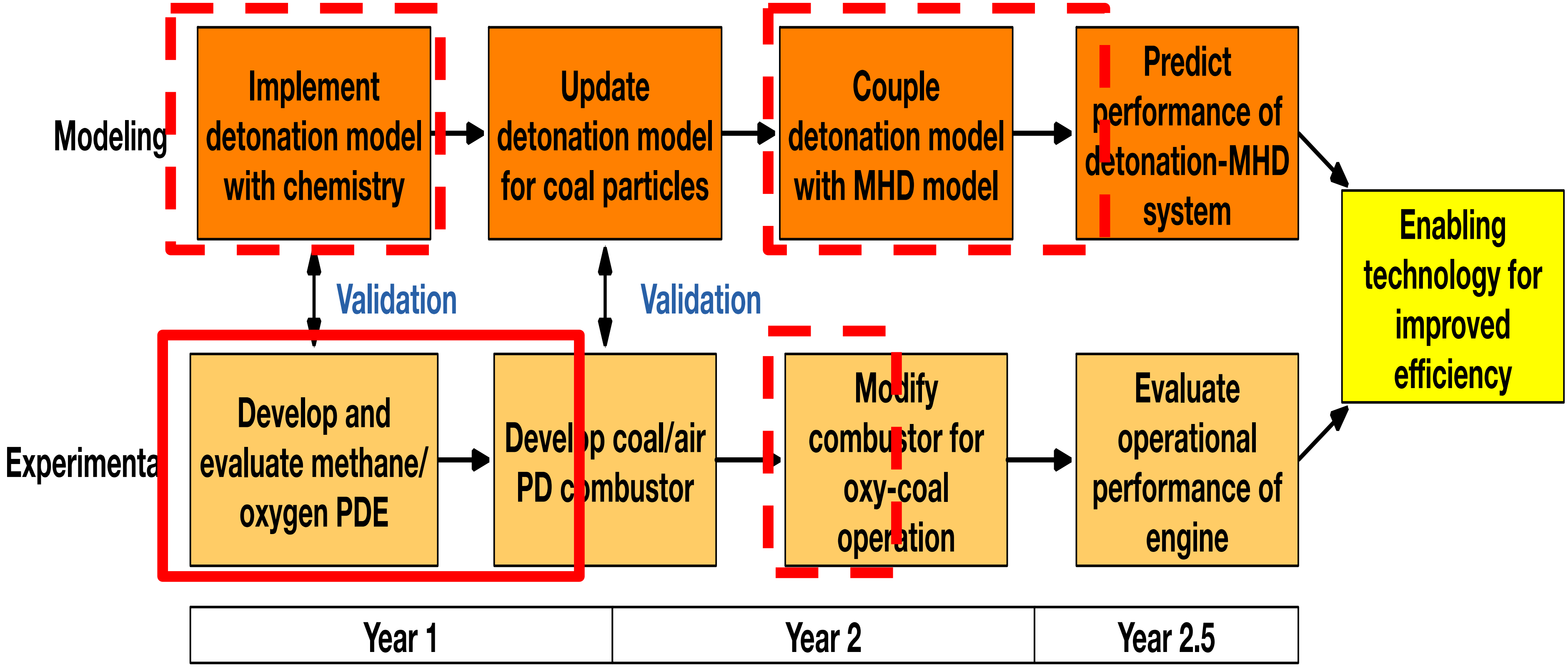
Overview of Tasks



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

Remainder of Talk

1) Develop Pulse Detonation Engine and Measure Boundary Condition (Task 2)
2) Development of Coal Seeder (Task 3)
3) Identification of Influence of CO_2 on Detonations (leverage effort with ONR)
4) Calculations (Task 4)
5) Future Work

Future Work

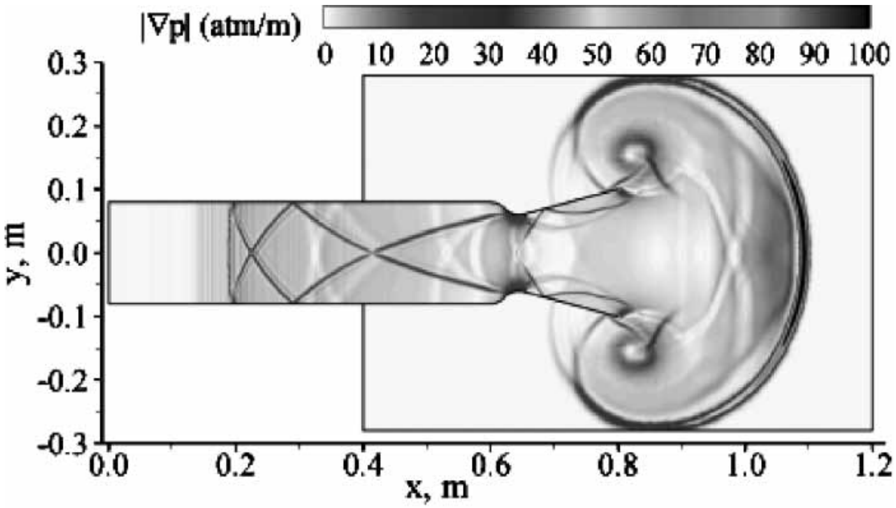
Experimental

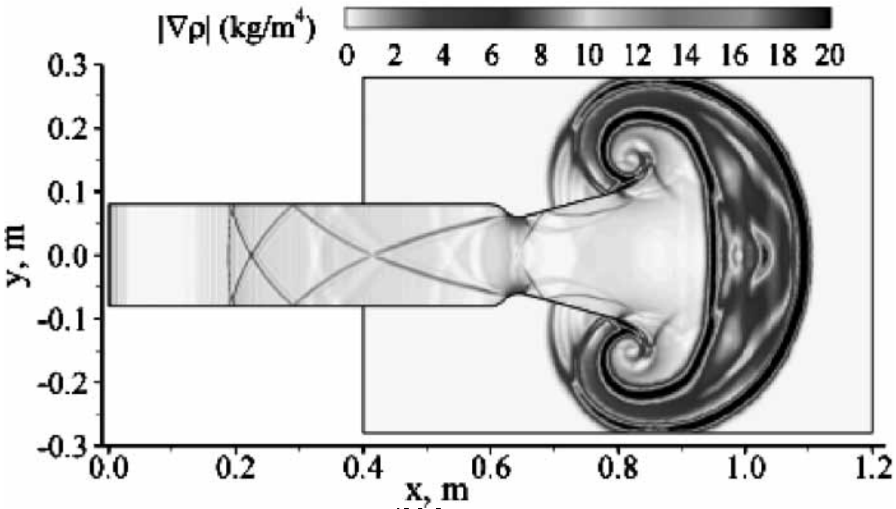
1) Transition PDE to operate using oxy-coal
2) Measure boundary conditions and velocities for calculations
3) Quantify changes in detonation characteristics between solid and gaseous fuels

Computational

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

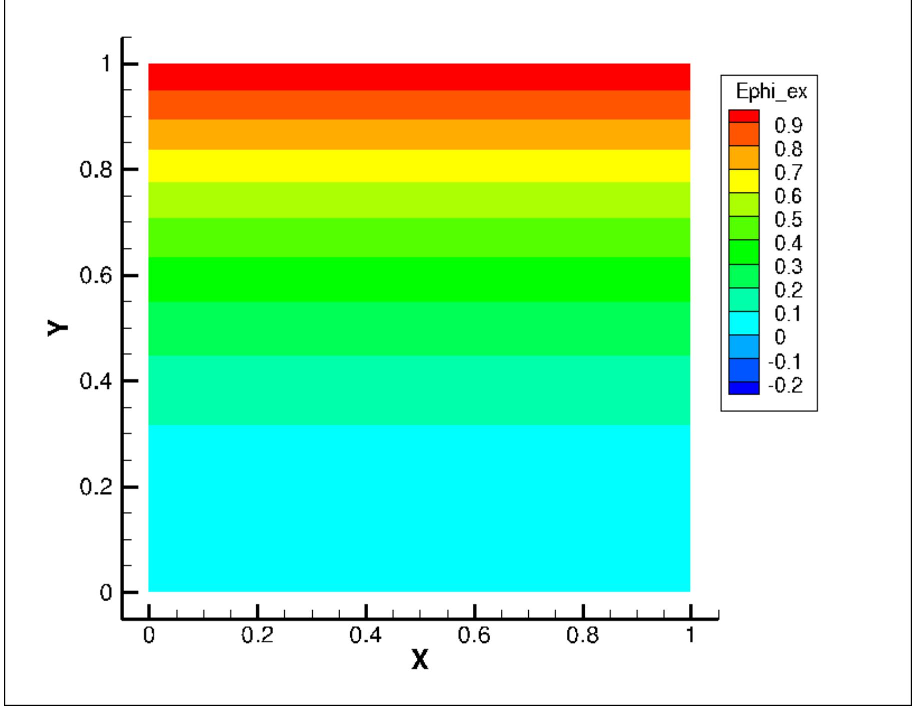
CE/SE Method: 2D Detonation Example



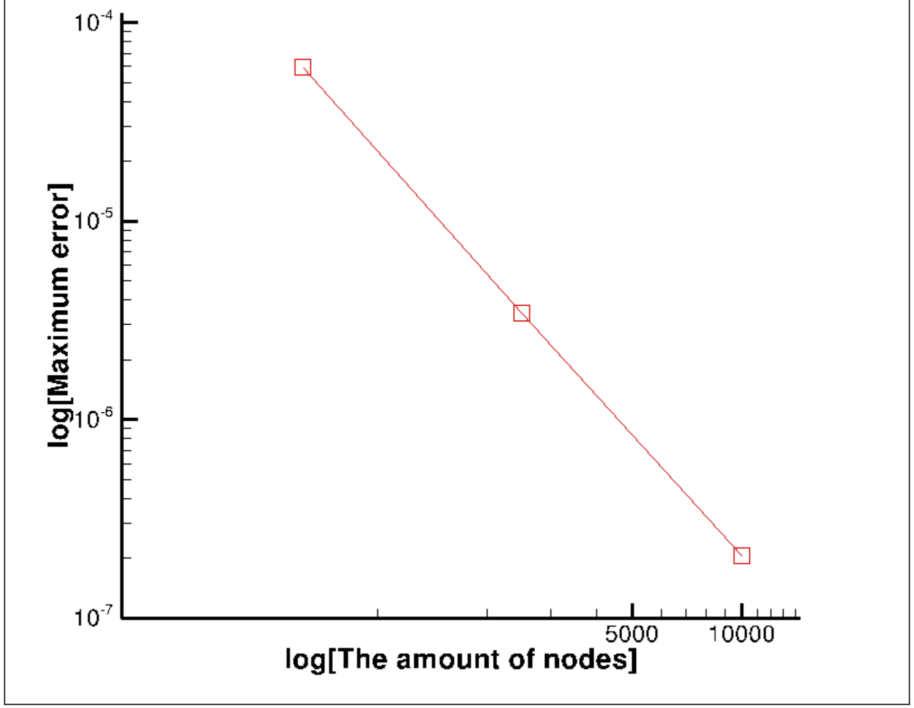


Wu, Ma, and Yang [14]

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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