Pulse Detonation Engine for Advanced Oxy-Combustion of Coal-Based Fuels

FE0025822

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Research Team

Dr. David L. Blunck

- Experimental reacting flow studies and radiative heat transfer, 3 years as researcher at Air Force Researcher including collaboration with pressure gain combustion group

Dr. Kyle Niemeyer

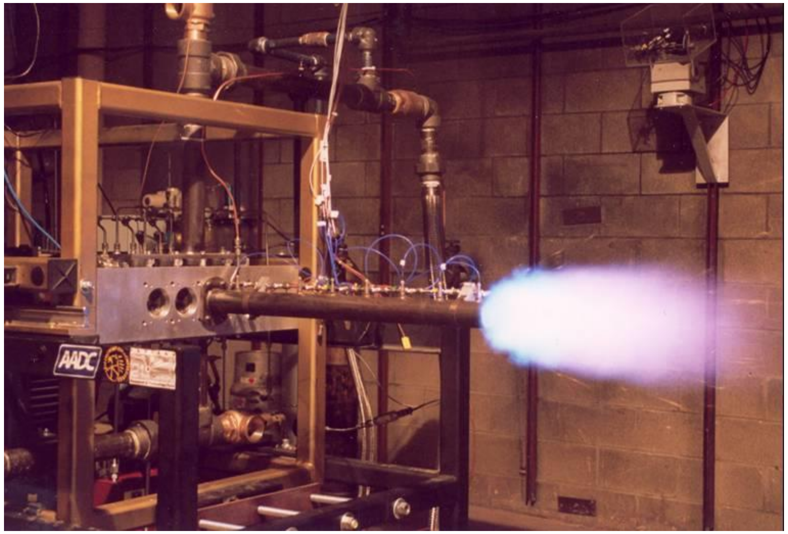
- Numerical combustion research and detailed chemical kinetics

Dr. Sourabh Apte

- Large eddy simulations, turbulence modelling

Motivation

- Improvements in thermal efficiency needed for power plants to address national energy challenges
- Pressure gain combustion can significantly improve efficiency
  - Pressure rise instead of pressure drop
  - Detonations often used
  - Unsteadiness of detonations challenging for turbomachinery



Pulse detonation engine firing [2]

- Magnetohydrodynamics can provide step increase in thermal efficiency (e.g., 60% as part of topping cycle [1])
  - Operates better with high velocity and high temperature flows
  - Extract power from flow prior to entering turbomachinery

Motivation

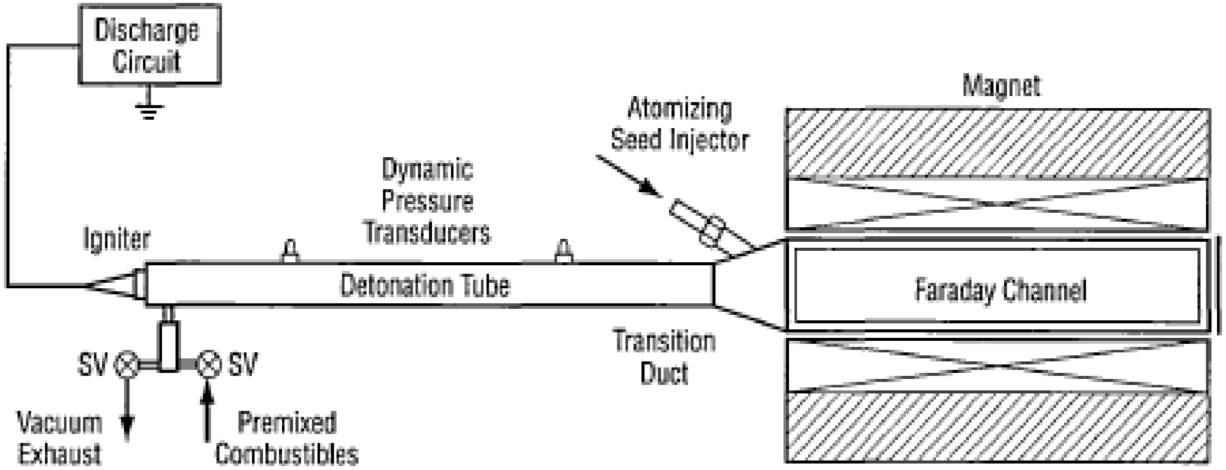


Illustration from prior detonation and MHD research [3]

- Prior (limited) research has considered detonations coupled with MHD, primarily for gaseous fuels
- Coal abundant resource in United States
- Little research investigating controlled detonations of coal (most research related to safety)
- Physical and thermal properties of coal detonations need to be measured to understand coupling with MHD

Technical Objectives

Overall Goal

The overall goal of the effort is to develop and evaluate a pulse detonation combustion system for direct power extraction, or magnetohydrodynamic (MHD) system, and expand the existing pool of data for model validation of MHD systems.

Specific Objectives:

1) Design, build, and operate a pulse detonation engine intended for use with a MHD application. The device operates on gaseous or solid fuels with oxygen as the oxidizer.

2) Evaluate the operational envelope and performance of the pulse detonation device with particular focus on the inlet design and the ability to operate with both seeded and unseeded flows Experimental diagnostics will include the ability to measure the effect of the fuel type, seed material and detonation wave on the electromagnetic properties of the reacted gas flow.

3) Develop and validate a numerical design tool to calculate the performance of pulse detonation and coupled detonation-MHD systems.

Technical Background: Detonations

- Supersonic flame front
- Detonation cells size characteristic of detonation properties
- High velocity ~ 2-3 km/s
- High temperatures ~3000K

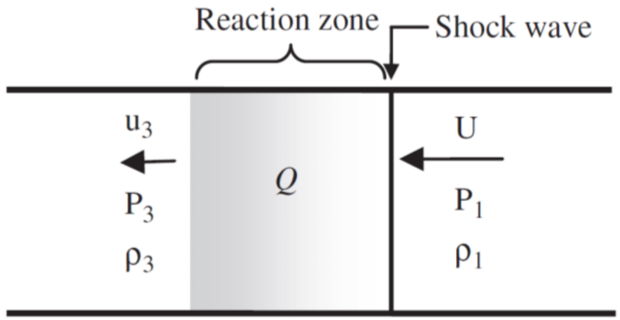
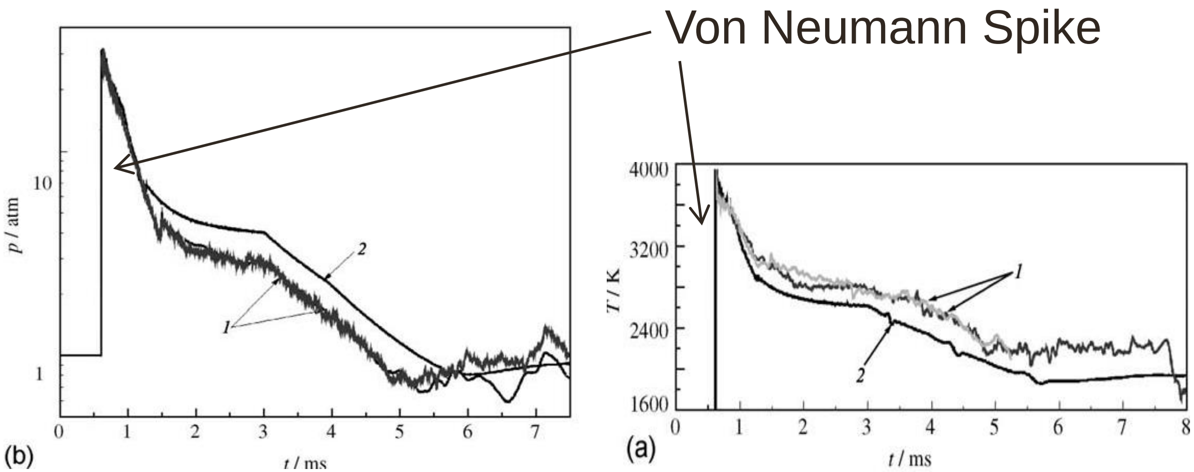


Illustration of detonation front [6]



Characteristic pressure wave [5]

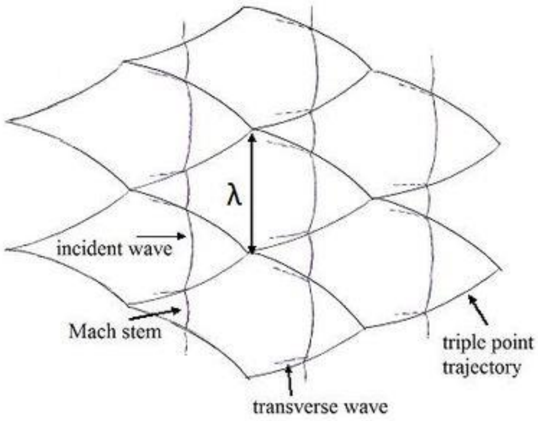


Illustration of detonation cells [4]

Pulse Detonation Engine

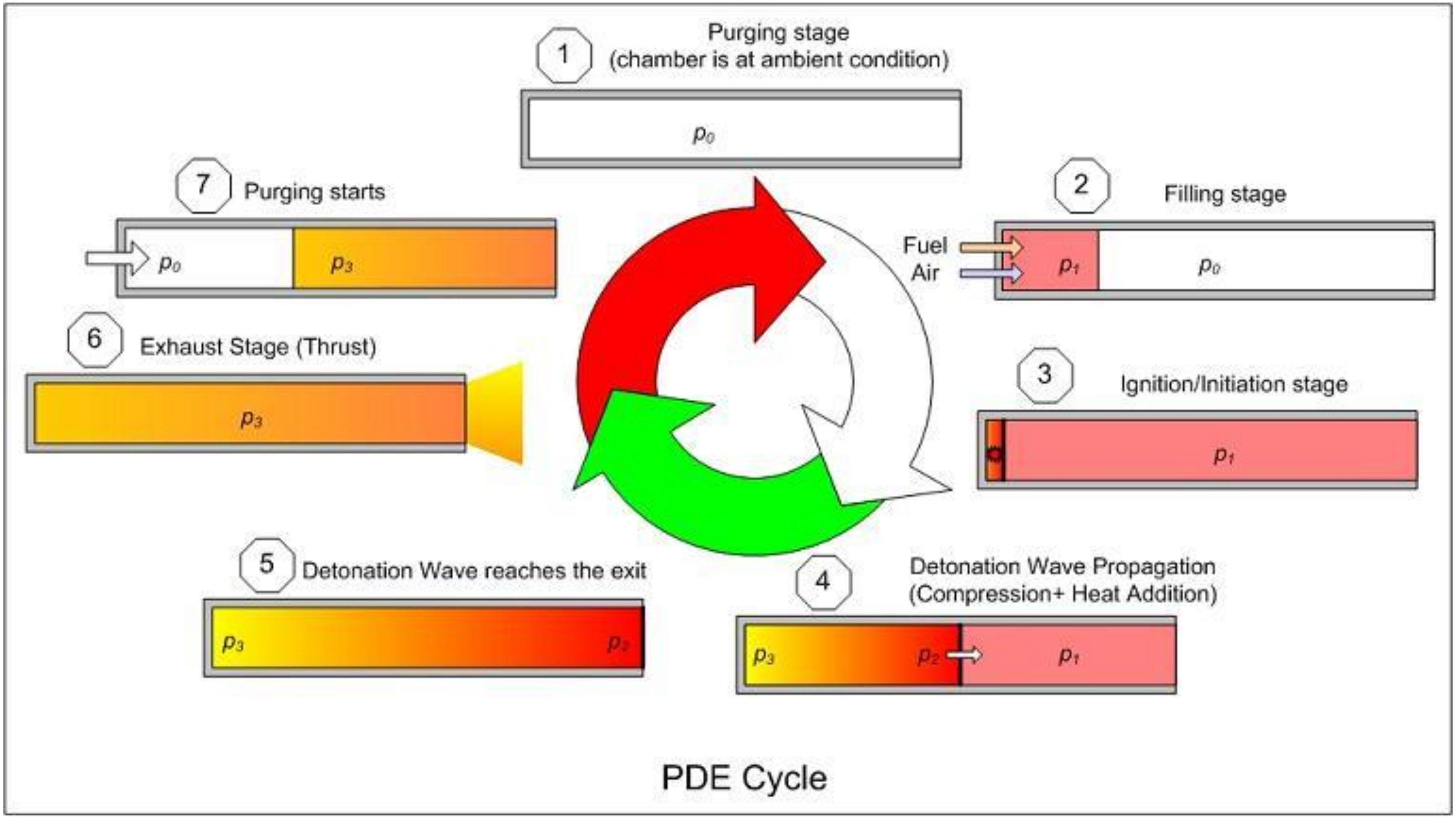
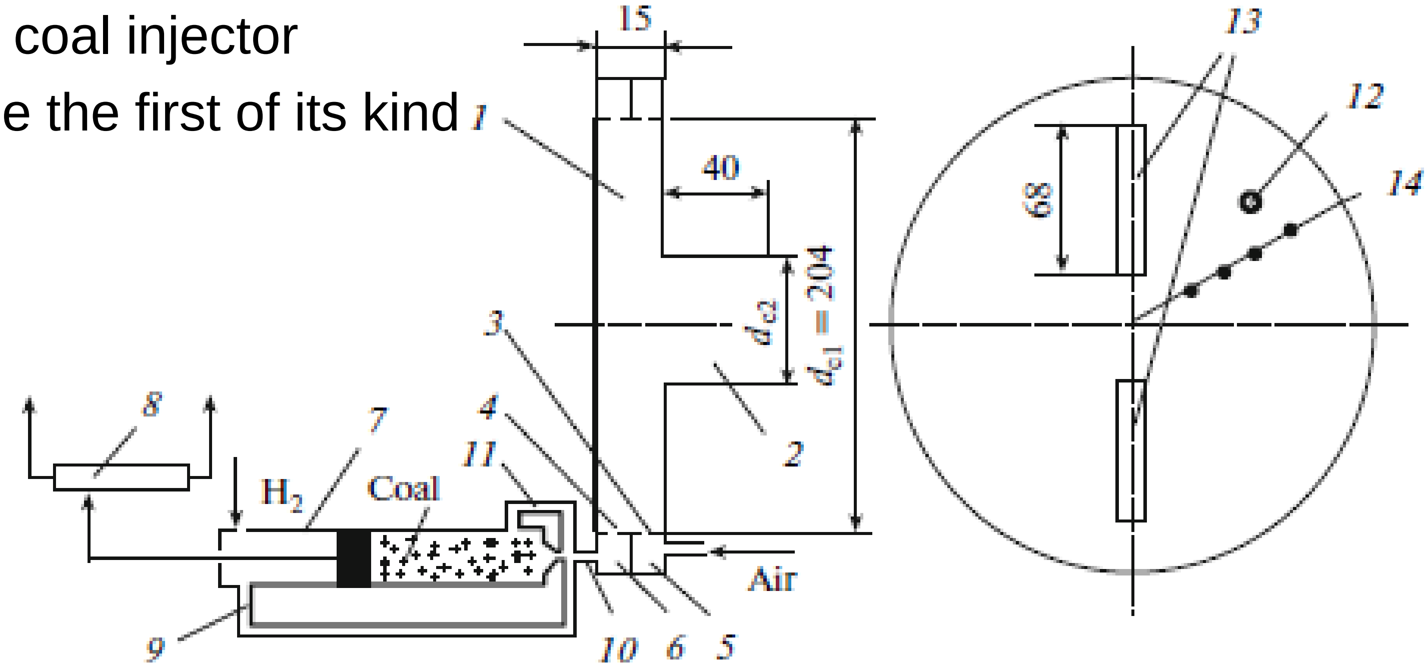


Illustration of pulse detonation cycle [7]

Coal Fired Pulse Detonation Engines

Work performed by F.A. Bykovskii et al. [8]

- H_2, air, coal
- 5–10 µm coal dust
- Syringe type coal injector
- Claimed to be the first of its kind



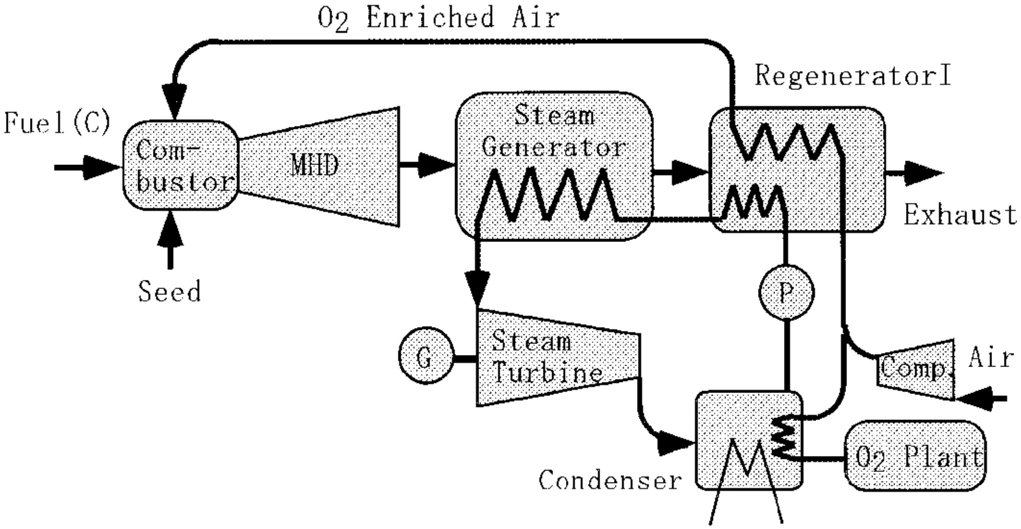
Method for feeding detonation tube with coal [8]

Technical Background: Computations

- Prior modeling studies on coal combustion at low speeds—limited or no detonation
- Prior studies on coupled detonation–MHD systems: major simplifying assumptions
    - Neglected coupled electromagnetic fields & fluid transport
    - Omitting detailed models for combustion chemistry
    - Simple one-step ionization reactions for seed material

MHD Power Generation

- Magnetohydrodynamic (MHD) power generation: electrically conductive fluid moving through a perpendicular magnetic field generates a current (*Faraday's Law of Induction*)
- Extracted power via MHD: $P \propto \sigma \times V^2 \times B^2$
- Previously investigated as topping cycle, coupled with low-speed coal combustion [9]



Challenge: low speed requires significant pressure drop to increase velocity

MHD Power Generation

- Potential benefits of detonation-fed MHD:
  - High velocities (Ma > 2) without pressure drop
  - High temperatures (T > 3000 K) increase electrical conductivity

- Prior research on detonation-MHD systems
  - Litchford et al. (NASA) & Cambier et al. (Air Force): MHD power extraction possible from propulsive PDE system [3,10,11]
  - Matsumoto et al. [12]: hydrogen-air PDE-powered MHD system
  - Major limitations:
    - Primarily propulsive systems; significant insight still needed into interactions between detonation and MHD field
    - Coal and natural gas significantly different than fuels studied (hydrogen)

CE/SE Methods for Pulse-Detonation

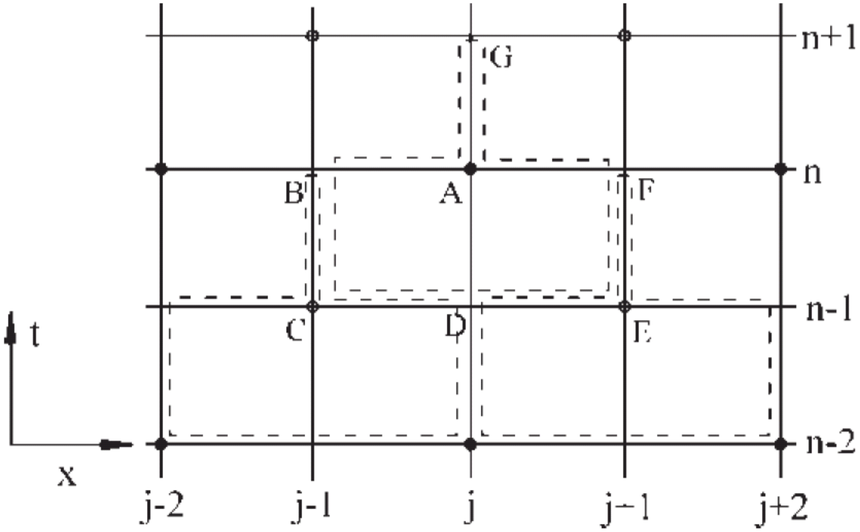
Basic approaches for reacting flows

- **Splitting Methods or Direct Methods**
  - Both approaches based on Total Variation Diminishing (TVD) or Flux Corrected Transport (FCT) concepts
  - Upwinding with approximate Riemann solver for face fluxes
  - Flux or slope limiters to avoid numerical oscillations
  - Complicated algorithms in multi-dimension
- **Conservation Element (CE)-Solution Element (SE) Method**
  - Chang et al. (1999) for non-reacting flows (NASA Glenn) [13]
  - Integral form of conservation equations in space-time
  - No Riemann solvers
  - Fluxes balanced through careful selection of conservation cell locations
  - Gradients of flow variables treated as independent unknowns
  - A compact, conservative approach; at least second-order in time
  - Subcycling for chemical reactions (Wu et al. 2004) [14]

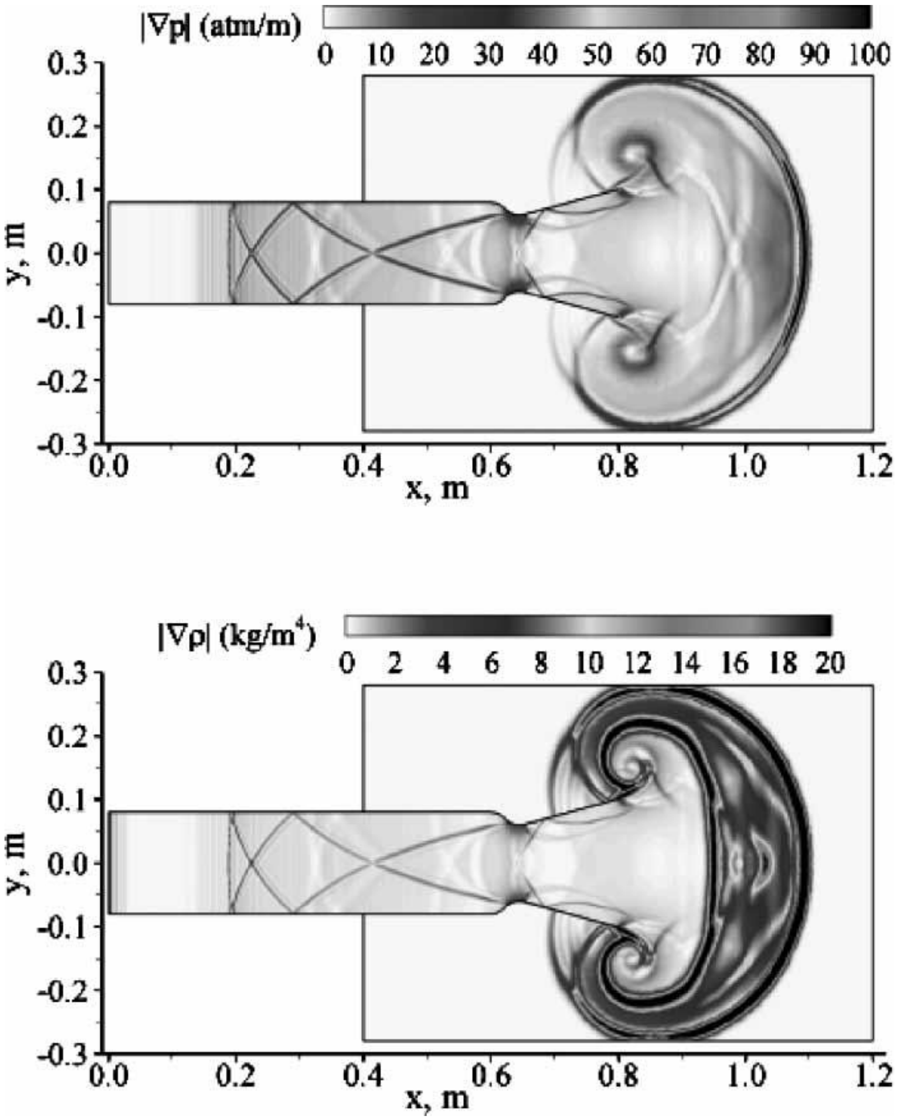
CE/SE Methods for Pulse-Detonation

- Apply integral form of equation on conservation element (area ABCDEFG shown on right)
- Base solver from Wu et al. [14]
- H_2–O_2 chemistry (9 species & 24 reactions; Franklach et al. [15])
- Validated for standard test cases
  - Incident shock-induced detonation
  - Stationary shock-induced detonation
  - 2D detonation
- Later used to study PDE flow dynamics and performance (Ma et al. [16–18])

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

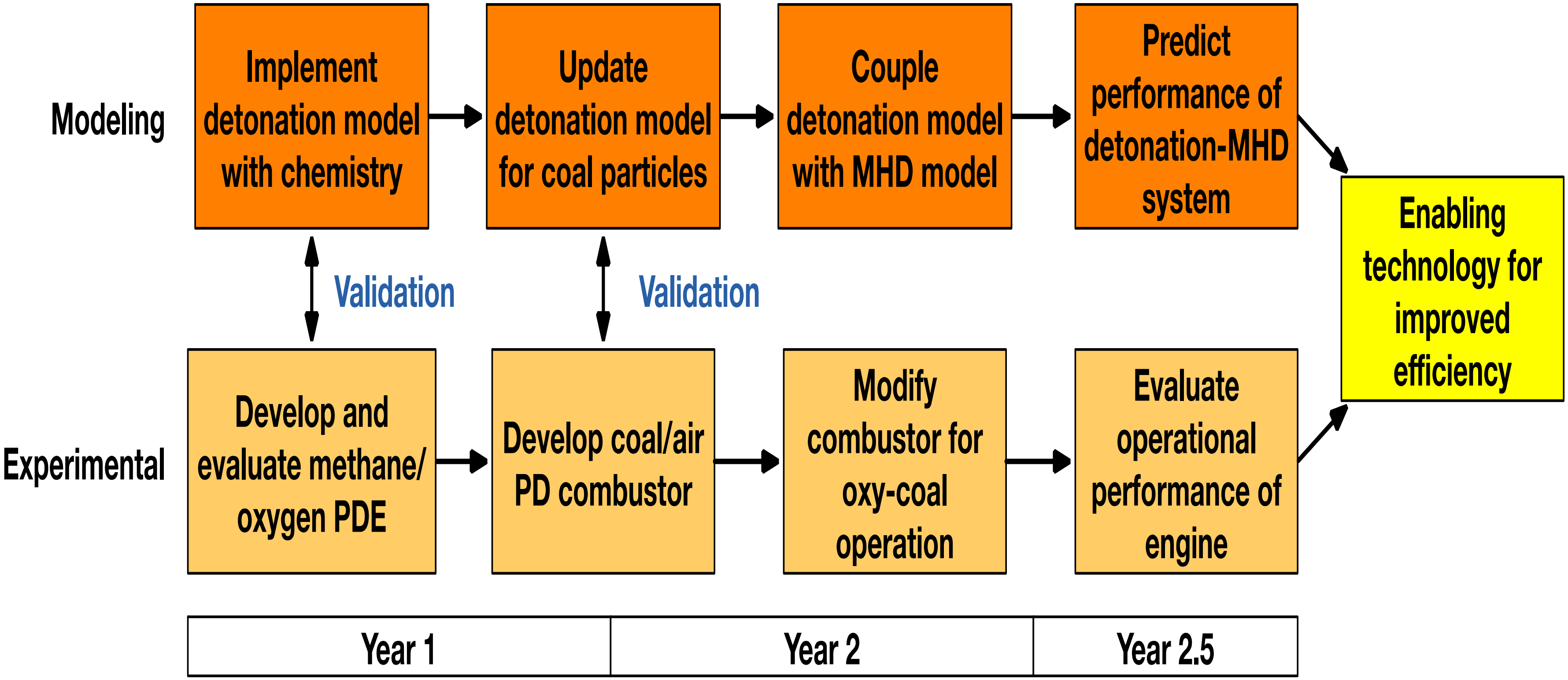


CE/SE Method: 2D Detonation Example



Wu, Ma, and Yang [14]

Overview of Research Approach



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

Research Tasks

1. **Project Management and Planning**
2. **Build and Evaluate Pulse Detonation Combustor which Operates on Methane-Air and/or Methane-Oxygen**
   - 2.1 Obtain design details and receive operational training
   - 2.2 Modify design for operation using oxygen and methane or gaseous fuels
   - 2.3 Build combustor and seeder
   - 2.4 Evaluative combustor performance
3. **Build and Evaluate Pulse Detonation Combustor which Operates on Coal and Oxygen**
   - 3.1 Modify design for operation using coal and air
   - 3.2 Build combustor for operation using coal and air
   - 3.3 Modify combustor for oxygen/coal detonations
   - 3.4 Evaluate combustor performance for coal detonations

Research Tasks

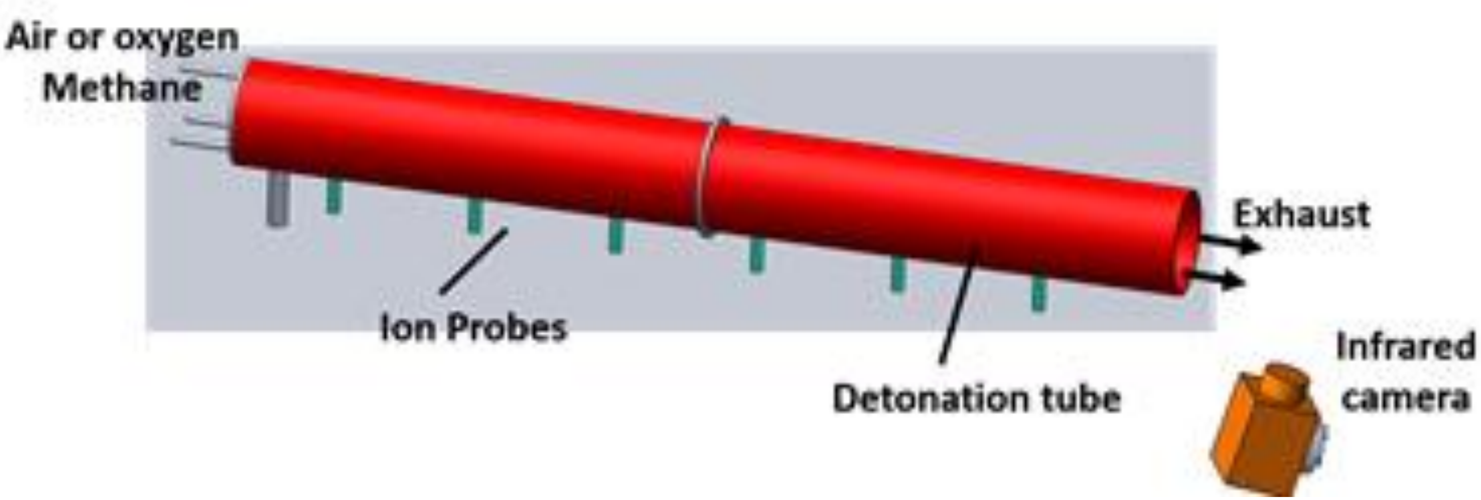
4. **Evaluate the Performance of a Coupled Pulse Detonation Engine and MHD Power Generator**

   4.1 Develop detonation code for oxy-coal

   4.2 Develop MHD physics solver

   4.3 Development and validation of a coupled oxy-coal detonation and MHD solver with parametric study

Task 2: Design and Build a CH_4/air/O_2 PDE

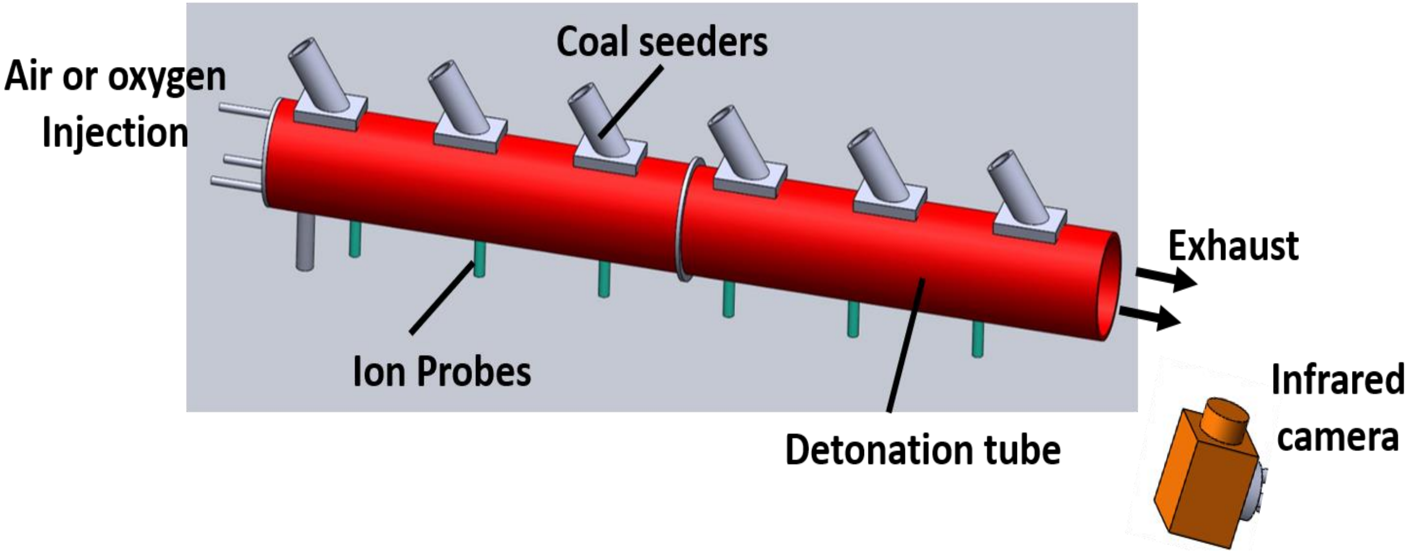


Task 2.1 – Visit AFRL (complete)

Task 2.2 – Design and Operate PDE on gaseous fuels and oxygen

- Predetonator design from AFRL used to initiate detonations
- Single shot detonation tube to be built initially
- Extend tube to involve continuous pulse detonations (e.g., 1 Hz)
- Care taken using O_2

Task 2: Design and Build a CH_4/air/O_2 PDE



Task 2.3 – Design, build, and integrate seeder

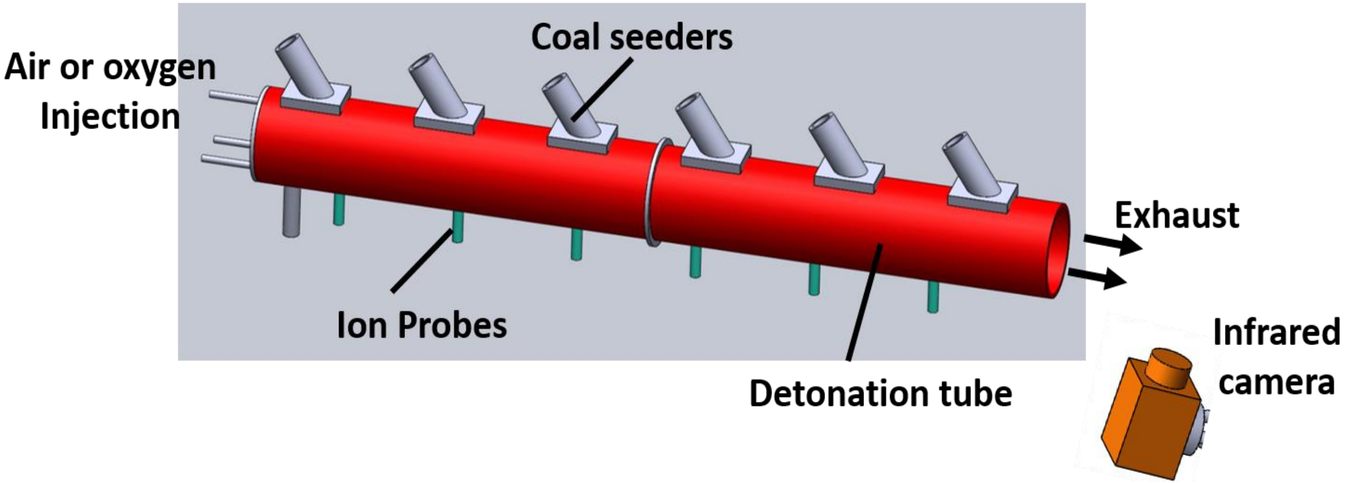
- Will seed flow to increase conductivity
- Will establish design for coal seeder
- Seek to create uniform seed addition
- Will quantify changes in detonation characteristics when seeding present

Task 2: Design and Build a CH_4/air/O_2 PDE

Task 2.4 – Evaluate detonation tube performance

- Operate detonation tube with and without seeding, at different fuel-to-air ratios
- Quantify operation envelop and any challenges
- Measure detonation speed using ion probes (design obtained AFRL) and electrical conductivity/resistivity of the flow (equipment borrowed from NETL if needed)
- Estimate exhaust temperatures using infrared camera
- Data to validate calculations and provide boundary conditions, provide insights into detonations at different seeding and operating conditions, insights into coupling with MHD

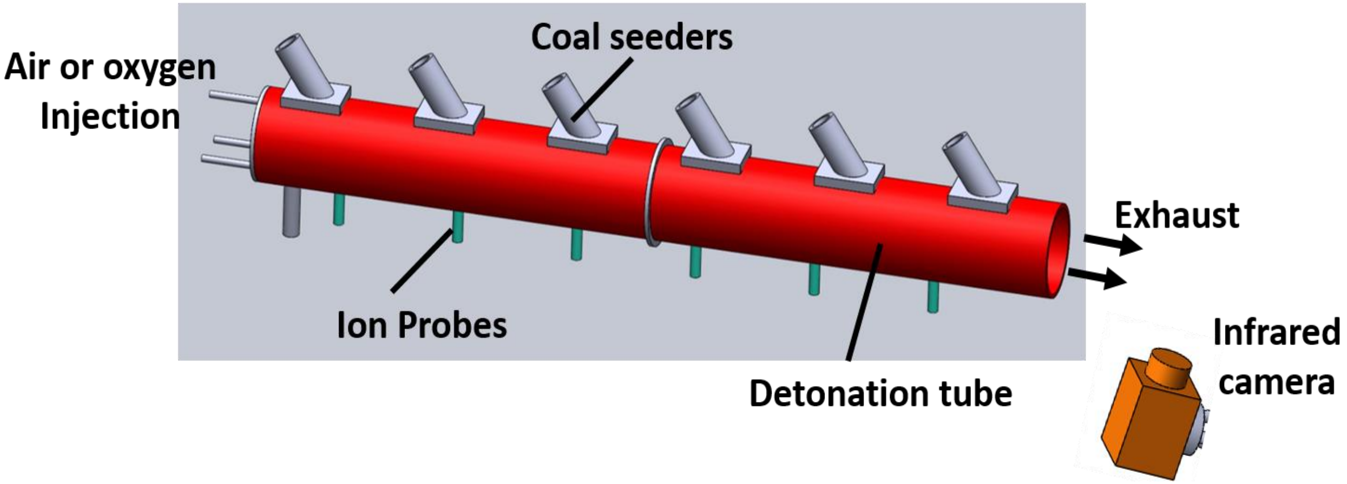
Task 3: Design and Build a Coal/air/O_2 PDE



Tasks 3.1 and 3.2 – Design and build combustor to operate using coal and air

- Modify or adjust seeder design as needed
- Calibrate flow rates and seed characteristics
- Coal powder to be used, well characterize for models
- Dilution with carrier gas may be required to reduce cell sizes
- Will seed with ionizing particles if needed

Task 3: Design and Build a Coal/air/O_2 PDE



Tasks 3.3 – Design and build combustor to operate using coal and oxygen

- Reduced cell sizes possible
- High exhaust temperatures will result
- Measure detonation speeds with air or oxygen
- Care when considering combustion with oxygen

Task 3: Design and Build a Coal/air/O_2 PDE

Task 3.4 – Evaluate detonation performance

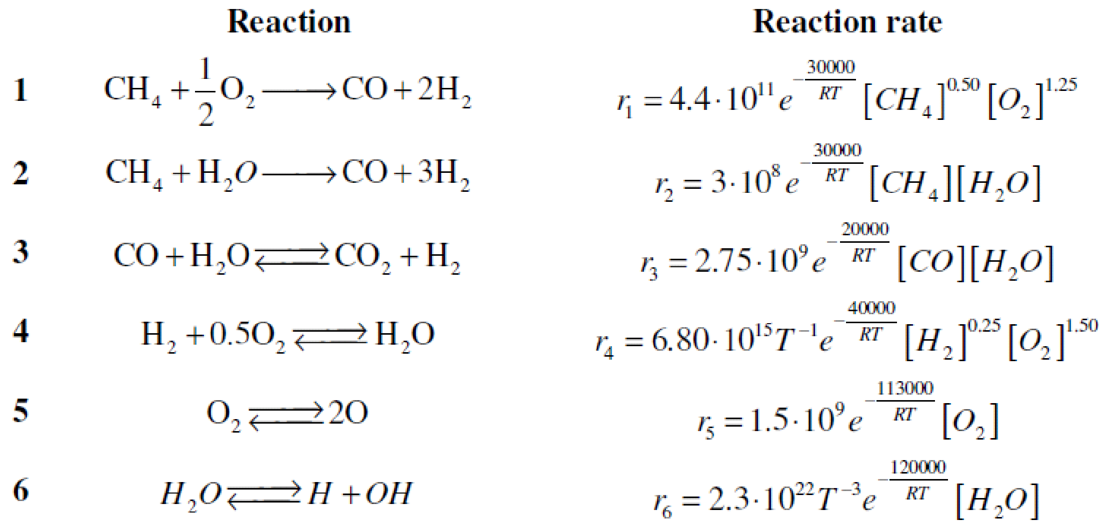
- Operate detonation tube with coal powder, at different fuel-to-air ratios
- Quantify operation envelope
- Measure detonation speed using ion probes (design obtained AFRL) and electrical conductivity/resistivity of the flow (equipment borrowed from NETL if needed)
- Estimate exhaust temperatures using infrared camera
- Data to validate calculations and provide boundary conditions, provide insights into detonations at different seeding and operating conditions, insights into coupling with MHD

Task 4: Calculate Detonation and MHD Performance

Task 4.1 Develop detonation code

- Convert the original CE/SE solver to Fortran 90 or C
- Incorporate simplified reduced reaction kinetics for oxyfuel combustion
- Implicit treatment and subcycling for reacting source terms
- Verification and validation against experiment

Jones-Lindstedt Mechanism with Dissociation Reactions (JL-R)



	Reaction	**Reaction rate**
1	$CH_4 + \frac{1}{2}O_2 \longrightarrow CO + 2H_2$	$r_1 = 4.4\cdot 10^{11} e^{-\frac{30000}{RT}} [CH_4]^{0.50} [O_2]^{1.25}$
2	$CH_4 + H_2O \longrightarrow CO + 3H_2$	$r_2 = 3\cdot 10^{8} e^{-\frac{30000}{RT}} [CH_4][H_2O]$
3	$CO + H_2O \rightleftarrows CO_2 + H_2$	$r_3 = 2.75\cdot 10^{9} e^{-\frac{20000}{RT}} [CO][H_2O]$
4	$H_2 + 0.5O_2 \rightleftarrows H_2O$	$r_4 = 6.80\cdot 10^{15} T^{-1} e^{-\frac{40000}{RT}} [H_2]^{0.25} [O_2]^{1.50}$
5	$O_2 \rightleftarrows 2O$	$r_5 = 1.5\cdot 10^{9} e^{-\frac{113000}{RT}} [O_2]$
6	$H_2O \rightleftarrows H + OH$	$r_6 = 2.3\cdot 10^{22} T^{-3} e^{-\frac{120000}{RT}} [H_2O]$

Frassoldati et al. [19]

Task 4: Calculate Detonation and MHD Performance

Task 4.2 Development of MHD solver based on CE/SE method:

- Two-dimensional equations (conservative form)

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0$$

$$\mathbf{U} = (\rho, \rho u, \rho v, \rho w, e, B_x, B_y, B_z)^T$$

F(U), G(U): flux vectors

↓

$$\nabla \cdot \mathbf{h}_m = 0, \quad m = 1, 2, \ldots, 8$$

$$\mathbf{h}_m = (f_m, g_m, u_m)$$

Transformed via Gauss' divergence theorem, then solved via standard CE/SE approach.

- One complication: need to ensure $\nabla \cdot \mathbf{B} = 0$
  - Follow extended CE/SE scheme proposed by Zhang et al. [20]
- Benchmark test cases:
  - Rotated one-dimensional MHD shock tube problem
  - MHD vortex problem

Task 4: Calculate Detonation and MHD Performance

Task 4.3 Couple CE/SE-based detonation and MHD solvers, perform parametric study of oxy-coal PDE-MHD power generation system

Necessary tasks:

- Develop coupled combustion & ionization chemistry model based on H_2-O_2 model of Schulz et al. [21]
- Add electron-impact ionization, electron-impact dissociation, associative ionization and charge-exchange reactions
- Addition of KO_2, KOH, KO, K, and single-step K ionization reaction

Validation against experiment:

- Detonation wave characteristics
- Properties of reacting/reacted flow with/without seed

Task 4: Calculate Detonation and MHD Performance

Task 4.3 Couple CE/SE-based detonation and MHD solvers, perform parametric study of oxy-coal PDE-MHD power generation system

Topics to be investigated:

- How much power can be extracted for different conditions?
- Effects of varying seed particle concentration, and determine optimum, for example Schulz et al. [21] found larger amounts of potassium seed interfered with detonation via radical competition
- Effect of fuel composition on detonation and MHD
- Explore possibility of seed-free operation through high detonation temperatures

Deliverables

- Fundamental understanding about velocity and conductivity of detonation waves with and without seeding (insight into potential for MHD coupling)
- Calculated MHD performance when coupled with detonation tube
- Understanding about achieving coal fueled pulse detonations
- Peer reviewed articles (4+ estimated)
- Program management plan
- As requested:
  - Detonation tube with operating instructions
  - Code developed for project (excluding code obtained from collaborator without permission)
- 3 MS/PhD students
- 4 undergraduate students with research experience (estimated)
- Final and mid-term reports

Experimental Facilities and Capabilities

Propulsion Laboratory

- Located near edge of campus
- Remote test operation in control room
- High speed DAQ being installed
- Student desks and space available

Picture within Propulsion Laboratory

Measurement capabilities

- Infrared camera (sensitive in mid-infrared, > 1 kHz possible)
- ICCD and high speed cameras available for measurements

Computational Facilities and Capabilities

- Existing computational model for gas-phase PDE to be obtained from collaborator
- Expertise in Finite Volume Methods (compressible and incompressible formulation) for reacting flows
- Access to CE/SE solver for compressible, reacting flows
- Experience in oxyfuel-combustion mechanisms
- Expertise in particle-laden, turbulent flows (Euler–Lagrange and Eulerian two-fluid approaches)
- In-house parallel computing cluster (built in collaboration with NETL), a high memory data processing server & access to OSU College of Engineering High-Performance Computing cluster

Collaborations and Synergies

Computational

- Interactions with Dr. Wu have been initiated to exchange the computational solver upon which the numerical modeling tool will be built
- Visiting graduate student from University of Tsukuba, Japan, with background in MHD simulations

Experimental

- Initial training and system design obtained from Innovative Scientific Solutions Inc.(ISSI)
- ISSI and Air Force Research Laboratory (AFRL) will continue to be a reference
- Dr. Rigel Woodside is building a MHD system at NETL in Albany, Oregon, will share results and use guidance

Progress to Date

- Received training and designs from AFRL
  - Received training related to PDE operation and safety
  - Designs for small detonation systems (pre-detonator)
- Revised predetonation design and acquiring materials
- Scheduled to have functional predetonation system by the end of the year (used to initiate detonations)
- Started designs for single shot detonation tube
- Specifying data acquisition system
- Laboratory prepared for detonation system
- Acquired a 1D solver based on Space-Time methods with reduced reaction chemistry
  - The solver is for single processor and Fortran 77. Needs an upgrade to Fortran90 or C.
- Currently recruiting graduate student for the computational part of the research

Potential Challenges

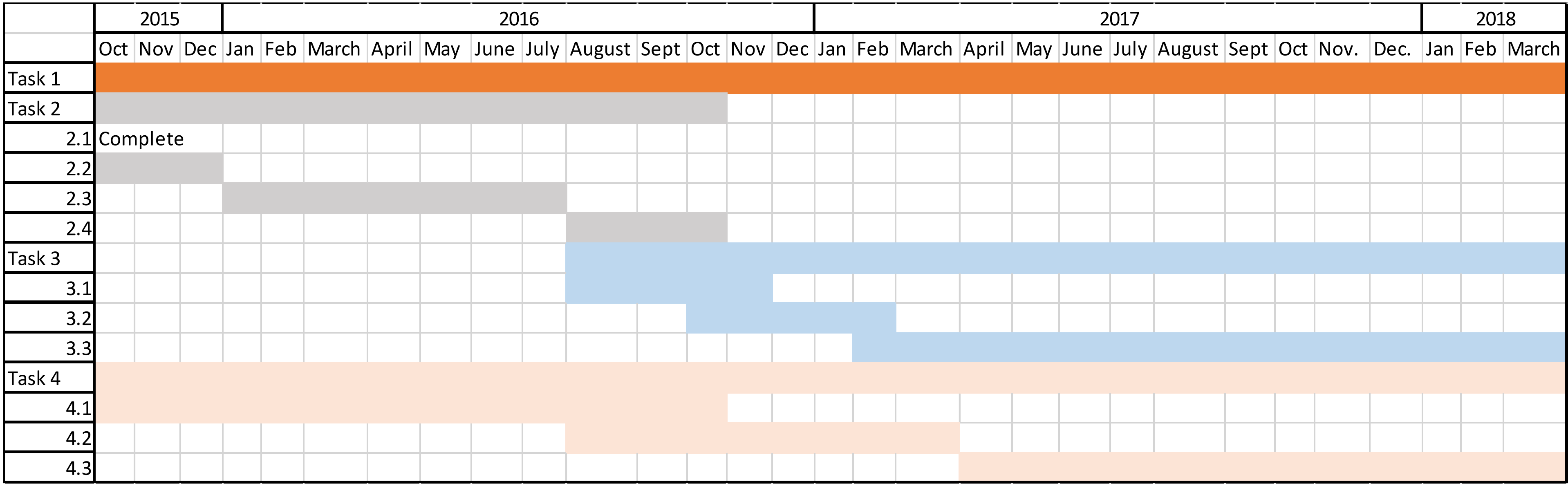
Experimental

- Valving and timing to achieve continuous operation, will work with AFRL as needed
- Coal – air has relatively large detonation cells, may require dilution with H_2 to achieve
- Coal feeding and distribution within detonation tube

Computational

- Coupling of flow dynamics and magnetohydrodynamics (space and time scale variations) – using CE/SE method should facilitate coupling
- Recruitment of graduate student – in progress

Timeline



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