DEVELOPMENT OF NOVEL COMBUSTION CODES FOR SUPERCRITICAL CO_2 COMBUSTION

8 Rivers Capital, LLC & National Renewable Energy Laboratory

HPC4EI Review Meeting Spring 2021

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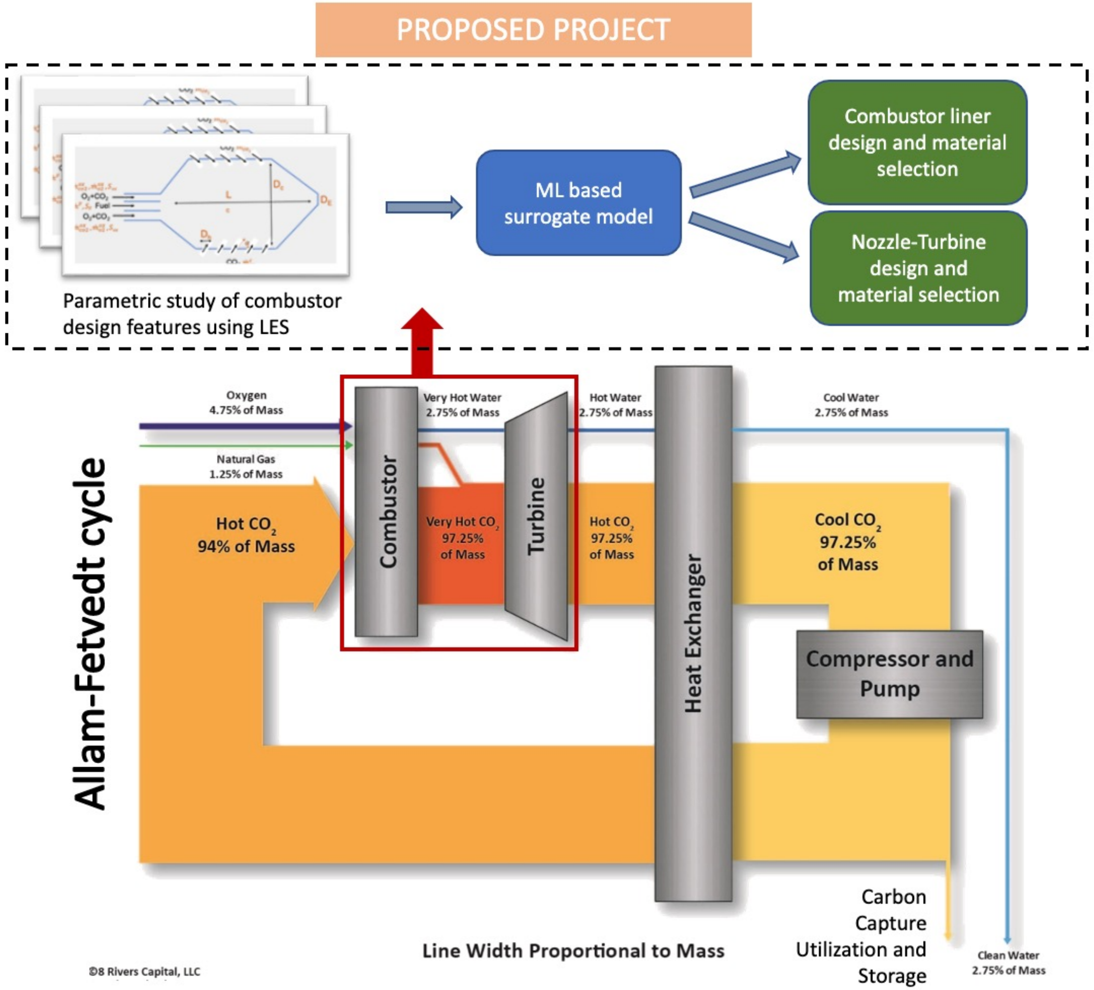
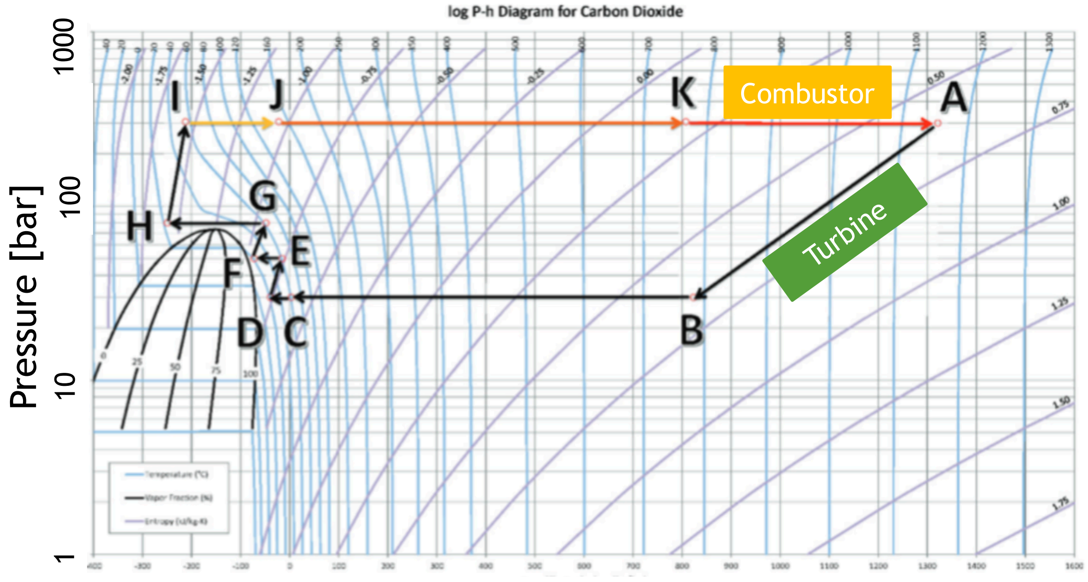
Project Summary



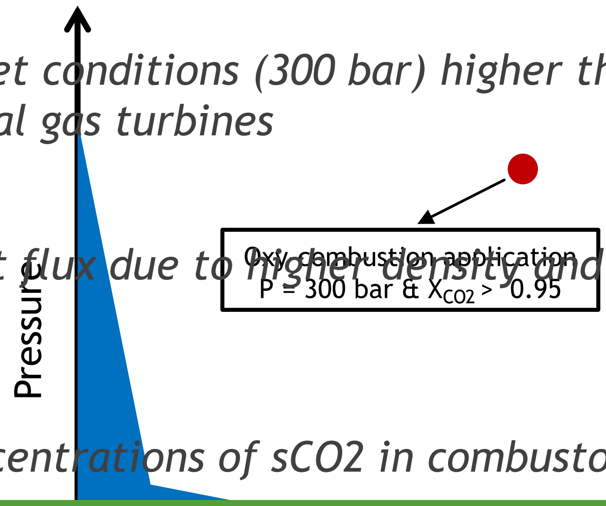
- *Allam-Fetvedt Cycle*
    1. *Novel supercritical CO2 (sCO2) power cycle developed by 8 Rivers Capital*
    2. *Critical technology – Combustor and Turbine interface*
    3. *Design and material selection one of the bottlenecks for deployment*
- *Develop a combustor surrogate model using high-fidelity reacting simulations*
- *Using surrogate model perform combustor liner and nozzle-turbine simulations to inform material selection*

Challenges & Opportunities

Simplified Allam cycle[1]



Combustor-Turbine conditions are unique compared traditional gas turbines



- *Turbine inlet conditions (300 bar) higher than conventional gas turbines*
- *Higher heat flux due to higher density and transport properties*
- *Higher concentrations of sCO2 in combustor exit*

Technology improvements needed over conventional gas turbines

1. Turbine and casing material
2. Thermal Barrier coating
3. Design of cooling technology for nozzles and turbine blades

1. Allam et. al, Energy Procedia, Volume 114, July 2017, Pages 5948-5966

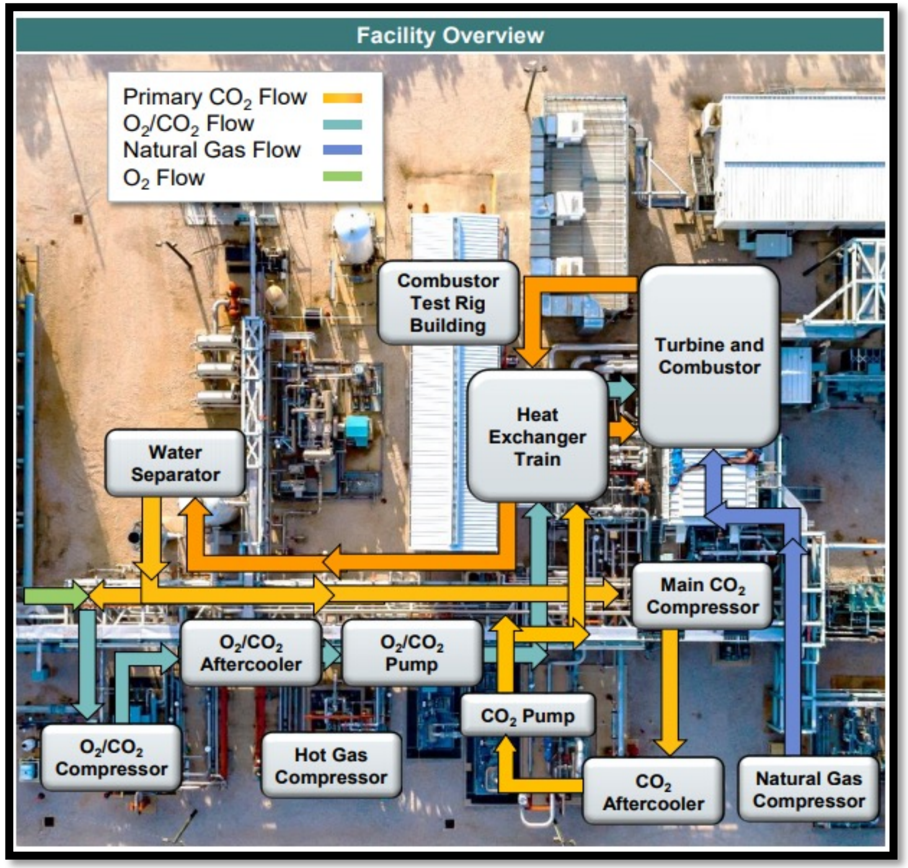
2. SWRI, Oxy-Combustion working group, https://www.netl.doe.gov/sites/default/files/netl-file/sCO2-WorkingGroup-Feb2018_1MWOxyCombustor.pdf

Industry Need

- *Commercializing the sCO_2 Allam Cycle requires new turbine combustor technologies. Being able to predict the conditions the combustor creates at the turbine inlet **critical** to system design.*
- *A $150M test facility in LaPorte, TX was developed by NET Power, a joint venture of Exelon, McDermott, Oxy Low Carbon Ventures, and 8 Rivers.*
  - *Toshiba "first of its kind" combustor tested in 2018, followed by plant-scale testing.*
  - *Commercial facilities are now in development across the world.*
- *The combustor has speed-to-market gaps, including few available test facilities (1 in the world), large investment/development requirements, and a lack of **validated, publicly available** CO_2 combustion CFD software.*

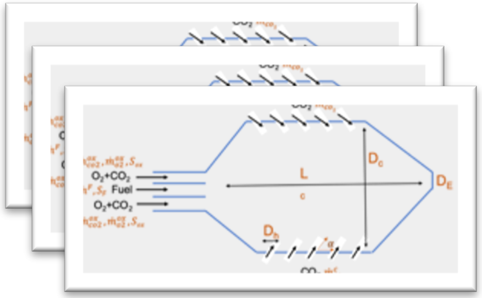
Using CFD as a virtual test-stand solves multiple problems:

- *Overall improvement of access to calibrated design tools.*
- *Allows multiple vendors to test designs with reduced cost and safety risk.*
- *Down-select designs before committing resources to physical testing.*



The NET Power AFC Test Facility, Photo Courtesy NET Power, LLC

Project Goals



Parametric study of combustor design features using high-fidelity simulations

ML based surrogate model

Combustor liner design and material selection

Nozzle-Turbine design and material selection

Highlight critical oxy-combustion characteristics & generate parametric dependence

Develop accurate and computationally in-expensive surrogate model

Design and material selection studies using surrogate model as a digital model for combustor

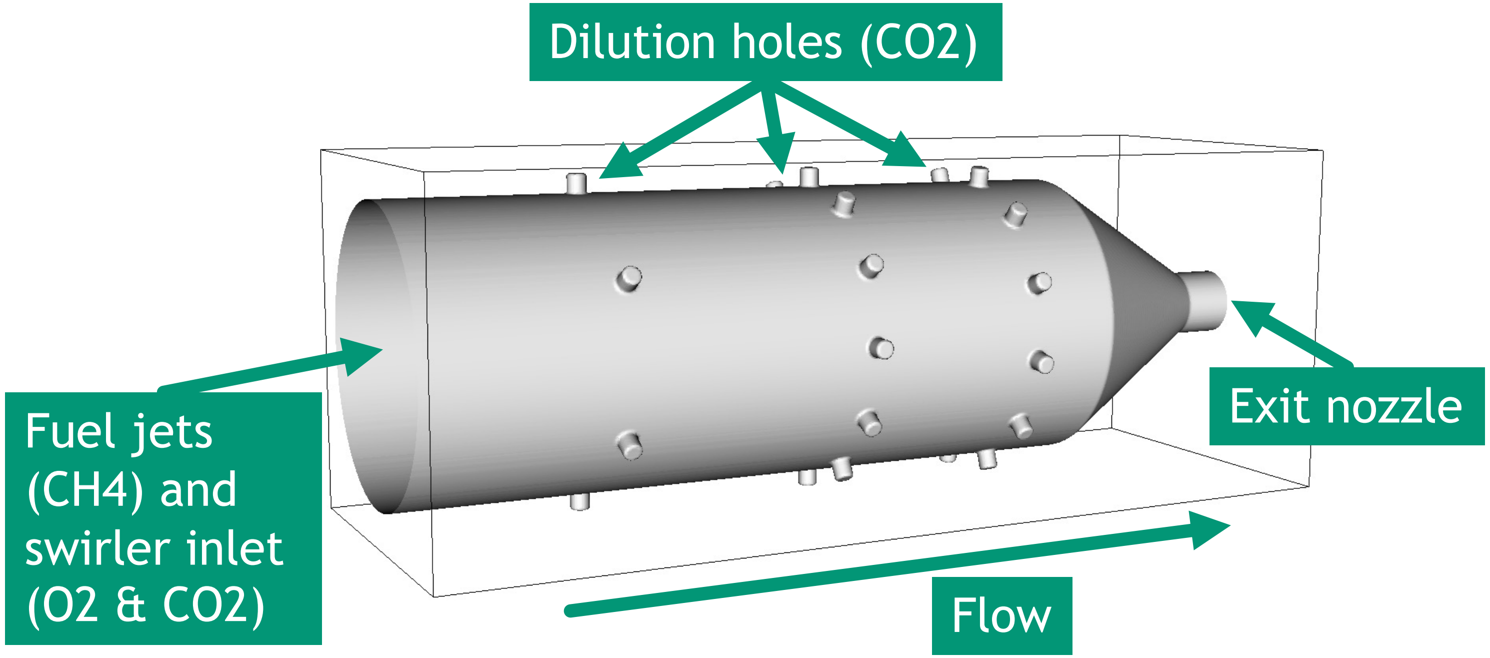
Petascale supercomputing resources - Summit at OLCF

Petascale supercomputing resources - Summit & Eagle (NREL)

Local workstations & smaller compute clusters available with industrial partners

Critical Technical Task

Task: High Fidelity Simulations of the Combustor



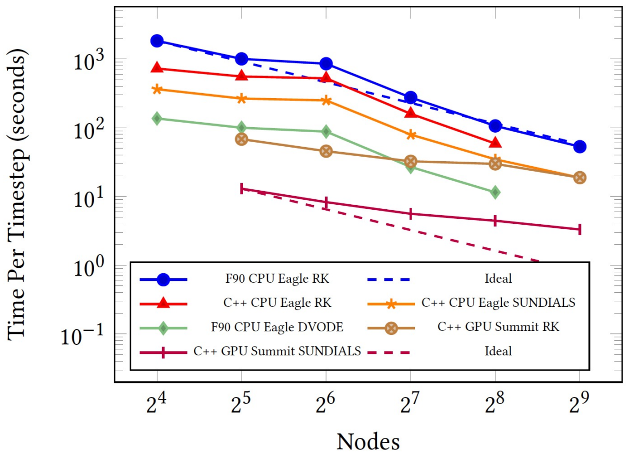
Major modeling challenges:

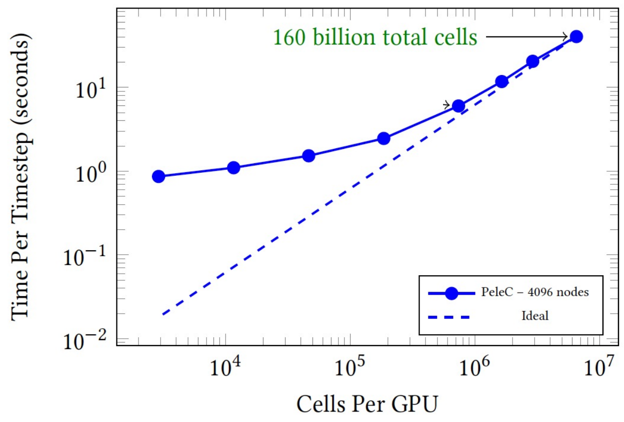
- Resolution of small-scale turbulence
- Complex multi-inlet geometry
- Non-ideal Equation-of-State
- Complex Chemical Kinetics

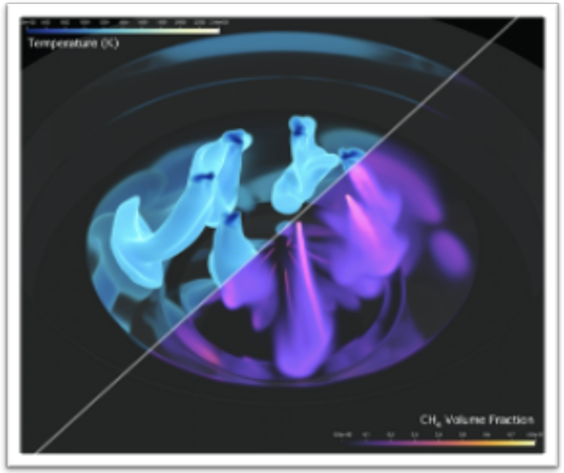
- *1. Couple of highly resolved simulations to interrogate critical physics phenomenon*
- *2. Parametric sweep of large eddy simulation (LES) to generate operating map based on key parameters*

Flow Solver - PeleC

PeleC strong scaling on multiple machines







Fuel jet impingement on piston bowl

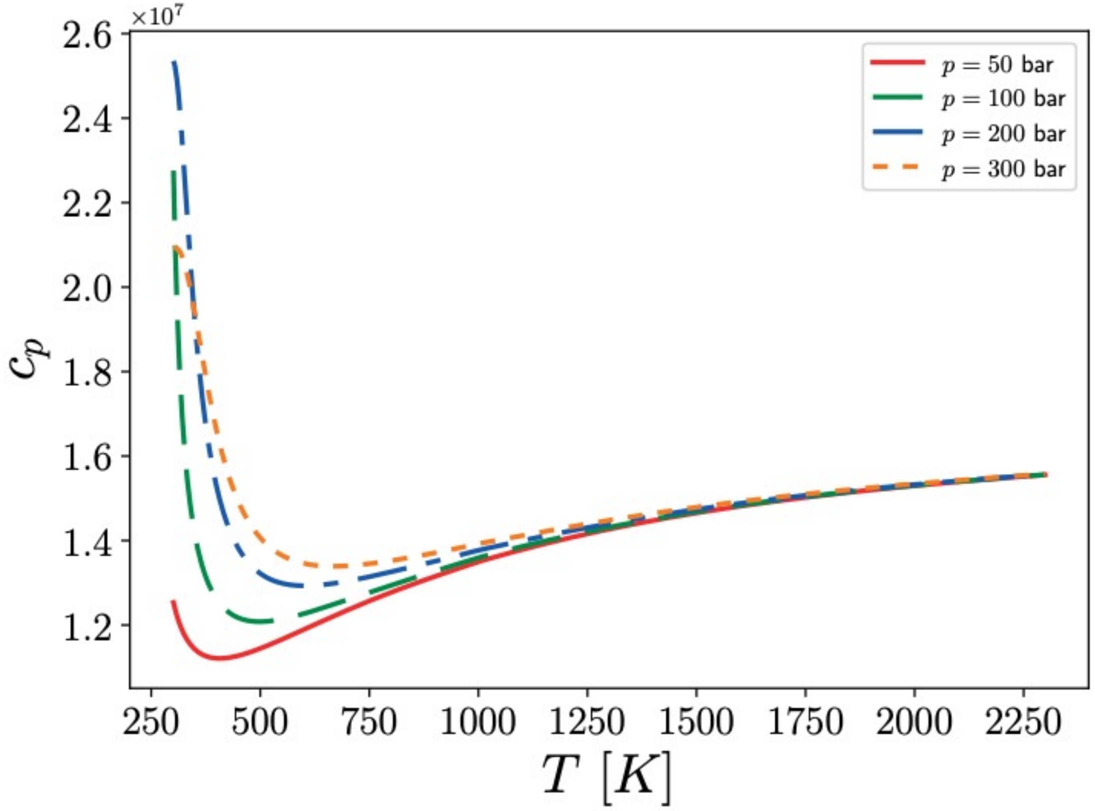
Fuel injection in supersonic cavity

- *PeleC: compressible reacting flow solver developed through Exascale Computing Project (ECP)*
  1. *Adaptive mesh refinement through AMReX library*
  2. *Complex geometry with embedded boundary treatment*
  3. *MPI/OpenMP + GPU Exascale ready code (Summit and early Exascale hardware)*
  4. *Complex physics: chemistry, non-ideal EOS for supercritical conditions*

Challenge – Non-Ideal behavior

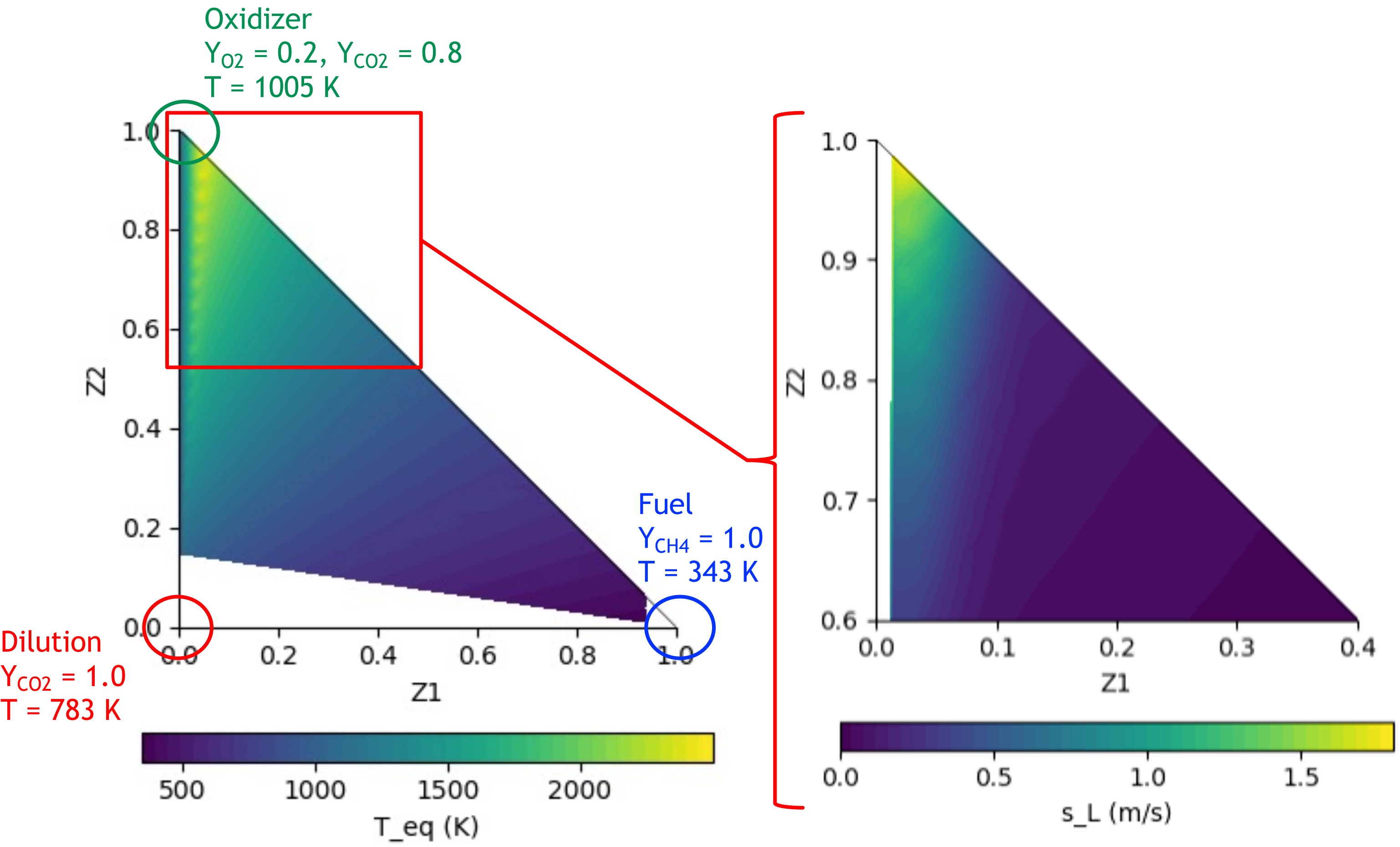
- *Non-ideal effects*
  - *Large variation in properties (e.g. large cp variations over the pressure and temperature ranges of interest)*
  - *We use the Soave-Redlich-Kwong EOS to solve for EOS quantities*
  - *Associated computational challenge for these capturing variations and solving a cubic EOS*
  - *Approximately 3-4x higher computational expense compared to ideal gas EOS (scales with N^2)*

Large variations for a stoichiometric CH4/O2/CO2 mixture



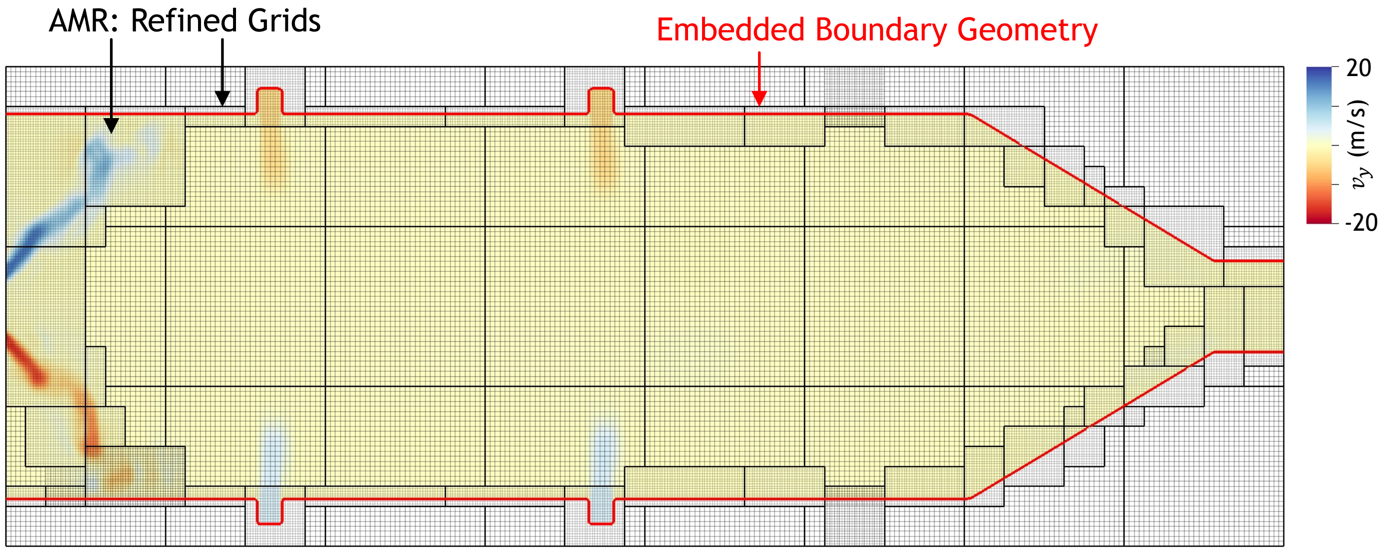
4. Sasaki et. al, Proceedings of the ASME 2017 Power Conference

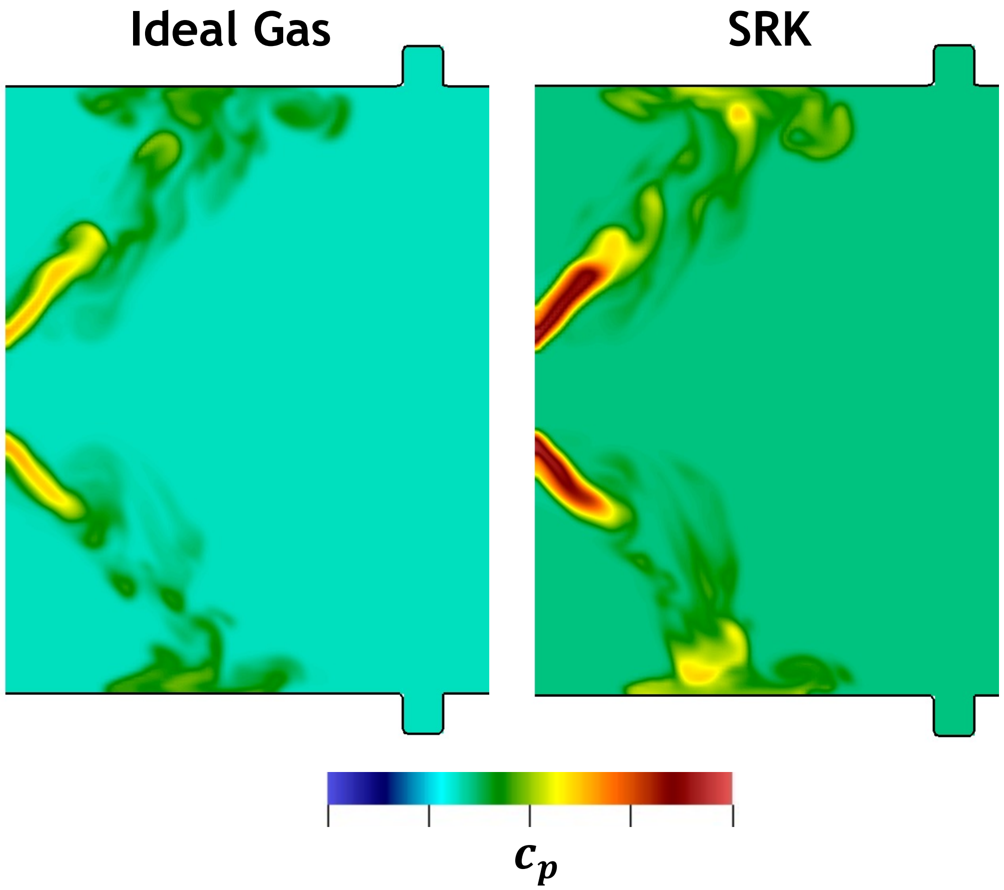
Challenge – CO_2 Concentration



- *Three-stream mixing between oxidizer, fuel, and dilution streams*
- *Combustion occurs with variable levels of CO_2 dilution and at varying temperatures*
  - *Presence of high-levels of CO_2 may change combustion process relative to traditional systems*
- *Premixed laminar flame speed varies significantly depending on the mixture*
  - *Key parameter for flame stability even in nonpremixed combustion*
  - *Low flame speeds at some conditions, particularly high dilution, may influence ability of flame to stabilize*
- *Prediction of mixing processes essential for accurate flame predictions*

Non-Reacting Flow

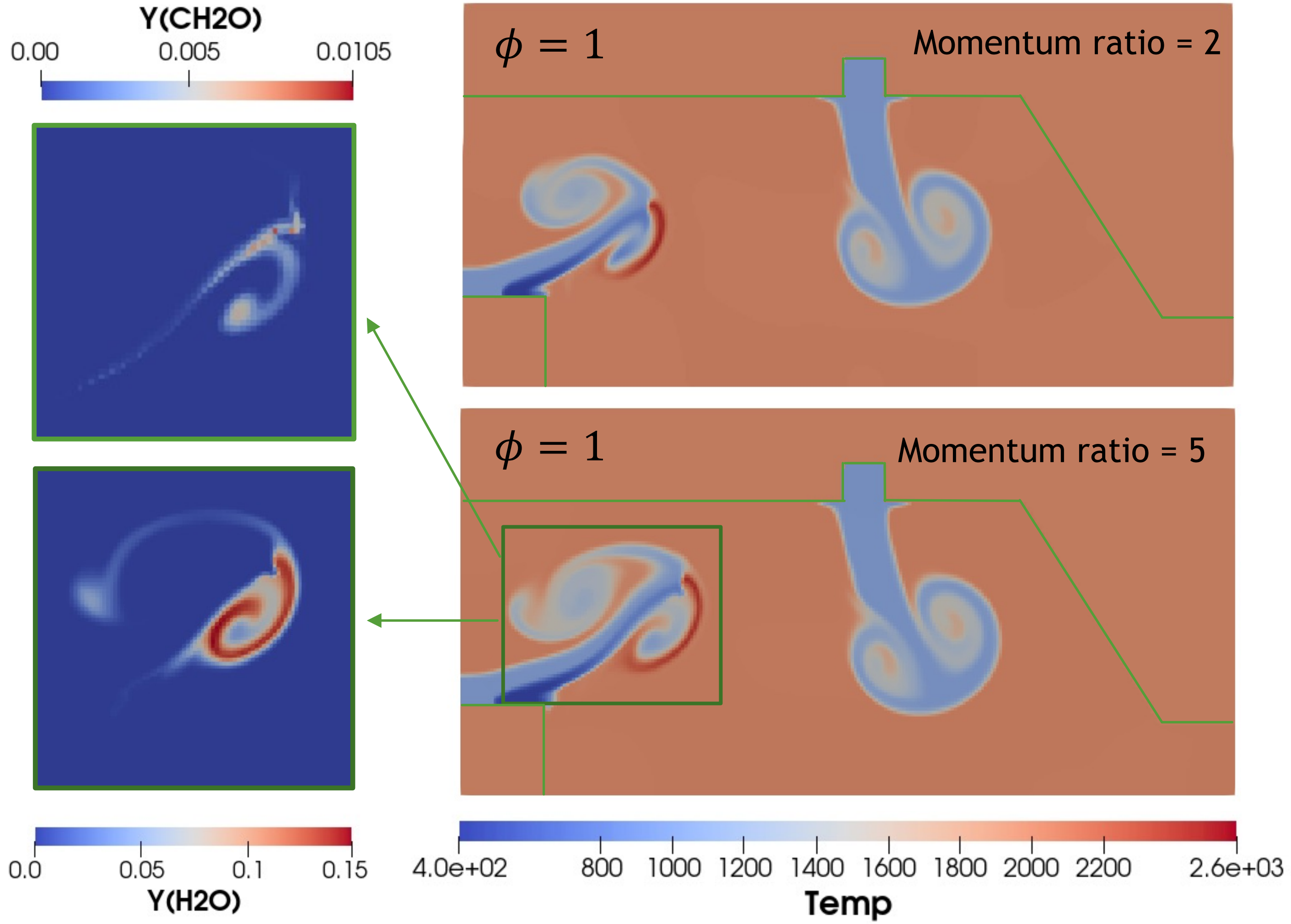




- *AMR: Finer grids resolve fuel jets, swirl, and EB representation of the geometry*
- *Significant difference in property calculations between ideal gas and SRK cases underscores the importance of the non-ideal EOS*

Reacting simulations – 2D

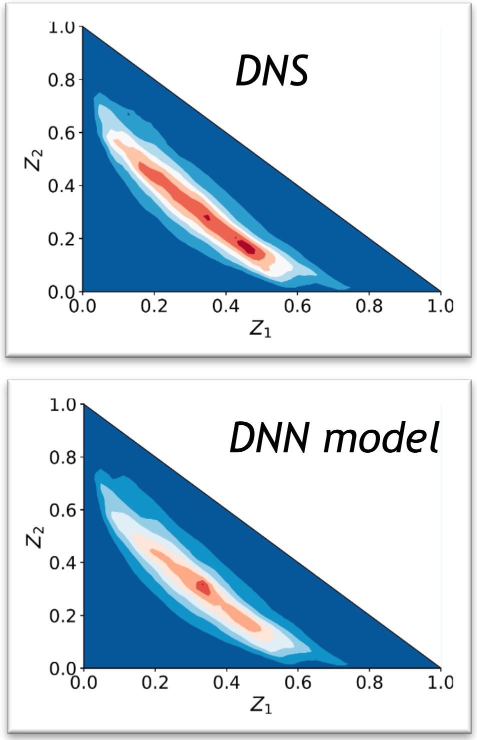
- *Parametric study*
  - *Momentum ratio* = $\frac{\rho_{oxidant}U_{oxidant}}{\rho_{fuel}U_{fuel}}$
  - *Working on defining parametric sweep*
  - *Initial simulations are promising*
  - *Ignition is observed at these conditions*
  - *This helps us define the right environment for 3D reacting simulations*



Next steps – simulations and surrogate model development

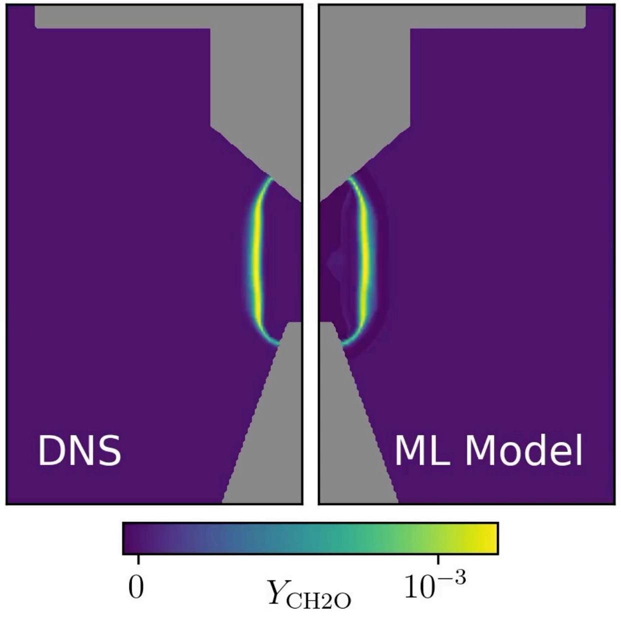
- *Applied Feb 2020, work started in Nov 2020 due to CRADA*
- *Perform parametric study using 2D and 3D simulations*
  - *Momentum ratio, equivalence ratio, geometry (e.g. number, size, spacing of dilution holes), swirl number*
  - *Generate large database of simulations using different configurations*
  - *Extract relevant data for input to surrogate model (inflow conditions, geometry, flow features)*
- *Develop surrogate model*
  - *Surrogate model to predict: pattern factor of temperature at the outlet, conversion CO/CO2 ratio, heat flux to the walls*
  - *Methods deployed:*
    - *Leverage existing expertise in model development*
    - *Bayesian approaches (e.g. Gaussian process regression) and DNNs*

Multi-scalar mixing



Yellapantula et al, 11th US NCM (2019)

DNN model for spark ignition



- Perform 2D and 3D parametric studies
- Develop surrogate model for relevant quantities of interest

Surrogate Model Application

- *Surrogate model developed at NREL*
  1. *Will be shared with 8 Rivers and their OEM partners*
  2. *Serve as boundary conditions for CFD and FEM analysis to study thermal stresses*
  3. *Study design of nozzle and blade cooling & combustor liner*
  4. *Study material selection for nozzle turbine assembly & combustor liner*
  5. *Computationally in-expensive to be used in workstations and small clusters available with industrial partners*

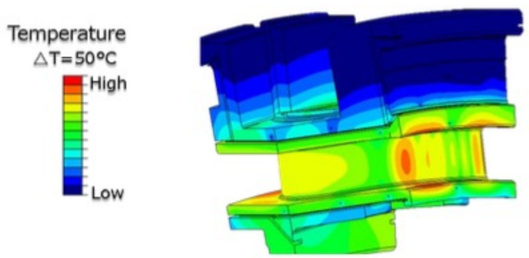


Figure 15: Metal Temperature Distribution for the First Stage Nozzle

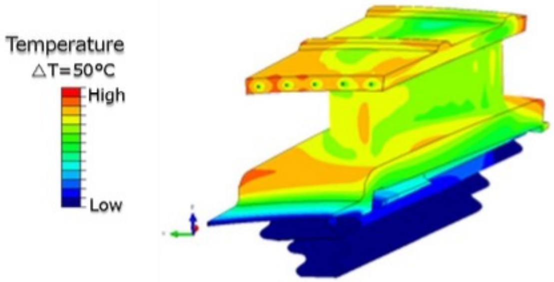
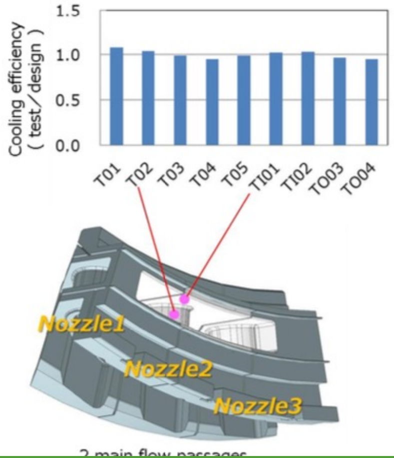


Figure 12: Metal Temperature Distribution for the First Stage Blade



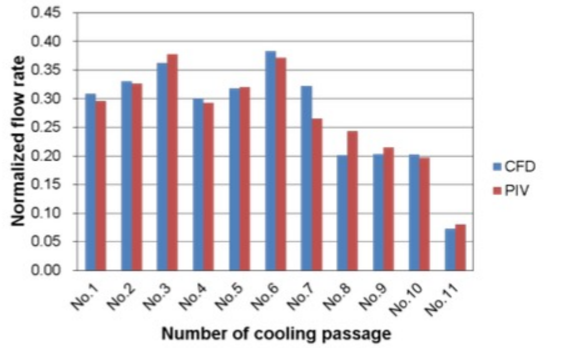


Figure 14: Comparison of Blade Cooling Flow Distribution

- NREL team will *d*emonstrate the workflow of using surrogate model
- Assist 8 Rivers and OEMs in using the surrogate model for design investigation and material selection

4. Sasaki et. al, Proceedings of the ASME 2017 Power Conference

Opportunities for leveraging project to support/foster future activities

- *Because this technology is crucial to 8 Rivers technology plans, 8 Rivers and NREL will explore continued collaboration, e.g. pursuing Phase 2 of this work*

- *SCO2 appears in multiple energy technologies of interest to DOE,*
  1. *Carbon Capture, Utilization, and Storage (CCUS)*
  2. *Concentrating Solar-Thermal Power (CSP), and High-Efficiency Heat Exchangers*
  3. *NREL will pursue opportunities to apply capabilities developed in this project to these technologies*

Acknowledgments

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