NREL
Transforming ENERGY

Influence of Real Gas Effects on Chemical Kinetics in Oxycombustion in Supercritical Carbon Dioxide

Mohammad Rahimi, Marc Henry de Frahan, Olga Doronina, Bruce Perry, Shashank Yellapantula, Ian Cormier, Marc Day, Michael Martin

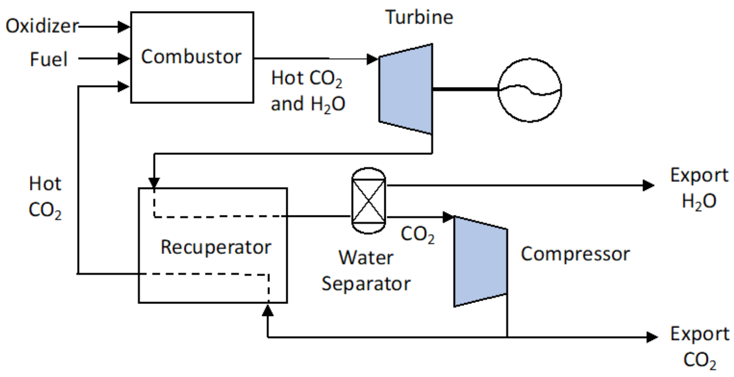
76th Annual Meeting of APS Division of Fluid Dynamics

Nov 19, 2023

Introduction

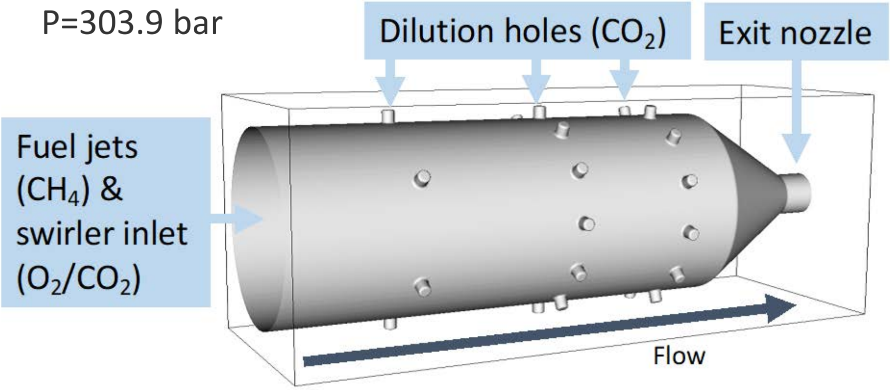
- The Allam Cycle offers the potential of electricity generation with zero carbon emissions by using oxy-fuel combustion in supercritical CO_2 working fluid.
- Recycled sCO_2 in the combustor (>90% mass):
  - lowering the combustion flame temperature
  - Diluting the combustion products
- Challenges for the design and material of the combustor (because of high T and P)
- Combustor simulation is also challenging because of non-ideal thermodynamics and transport properties.

Simplified Allam Cycle Schematic



Simulation Method

- Simulations used PeleC, a compressible reacting flow code based on AMReX framework.[1]
- 2nd order finite volume, 2nd order explicit Runge-Kutta time integration.
- Embedded boundary for complex geometry
- Ideal gas and Soave-Redlich-Kwong real gas EOS
- UCF Chemical Mechanism (16 species) used for supercritical CH4/O2/CO2 mixtures.[2]
- Domain is 25 x 8 x 8 cm
- Mesh is 256 x 96 x 96 with additional 3 levels of Adaptive Mesh refinement
- (0.1 - 1 mm cell sizes) ~ 82 mil cells



Inlet	Composition	Temperature	Velocity
Fuel jet	40-100% CH_4, 0-60% CO_2	343.15 K	64.47 m/s
Oxidizer swirler	80% CO_2, 20%O_2	1005.35 K	45.133m/s (axial), 54.16m/s (azimuthal)
Dilution holes	100% CO_2	783.15 K	47.09 m/s (wall normal)

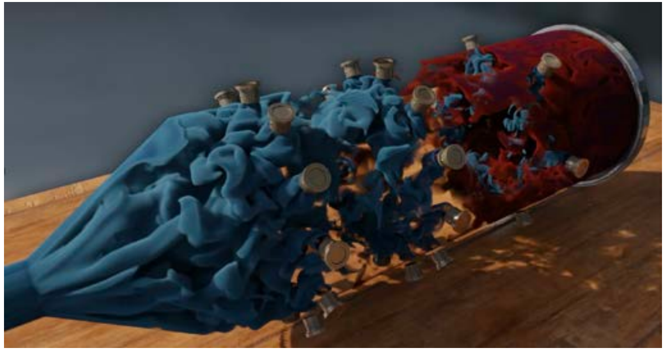
[1] Henry de Frahan, M. T., et al (2023). PeleC: An adaptive mesh refinement solver for compressible reacting flows. The International Journal of High Performance Computing Applications, 37(2), 115-131
[2] Manikantachari,Vesely,Martin,Bobren-Diaz,Vasu,S(2018). Reduced chemical kinetic mechanisms for oxy/methane supercritical CO2 combustor simulations. *Journal of Energy Resources Technology*, *140*(9), 092202.

Study Cases

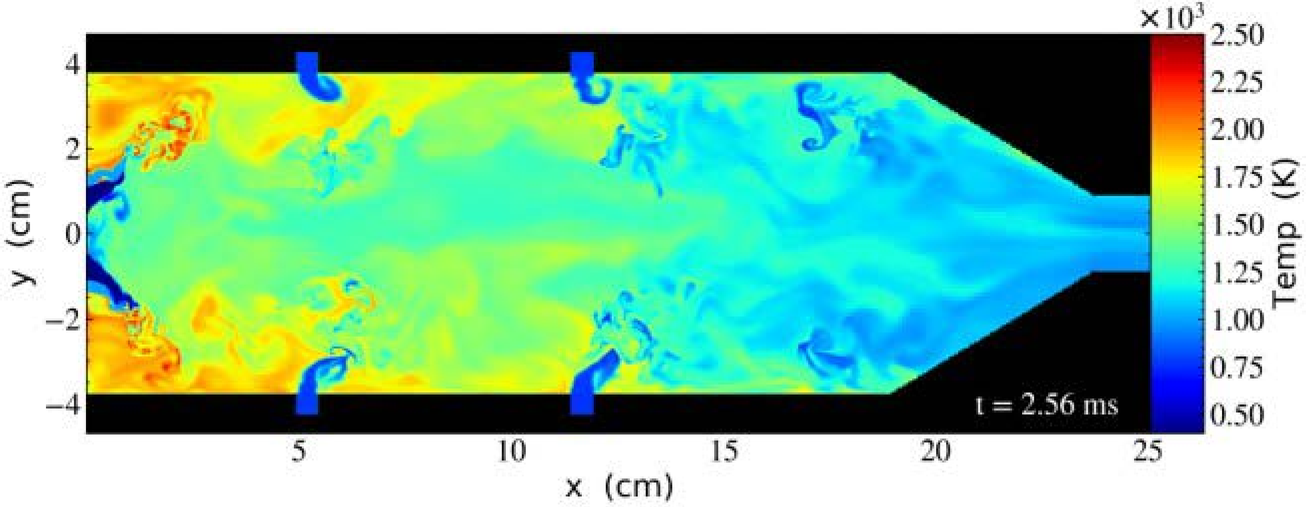
4 cases run using 80 nodes (6 GPUs per node) on Summit, using about 200,000 node hours.

Case	Fuel jet composition	Equation of state
1	100% CH_4	Soave-Redlich-Kwong (SRK)
2	100% CH_4	Ideal Gas
3	40% CH_4, 60% CO_2	Soave-Redlich-Kwong (SRK)
4	40% CH_4, 60% CO_2	Ideal Gas

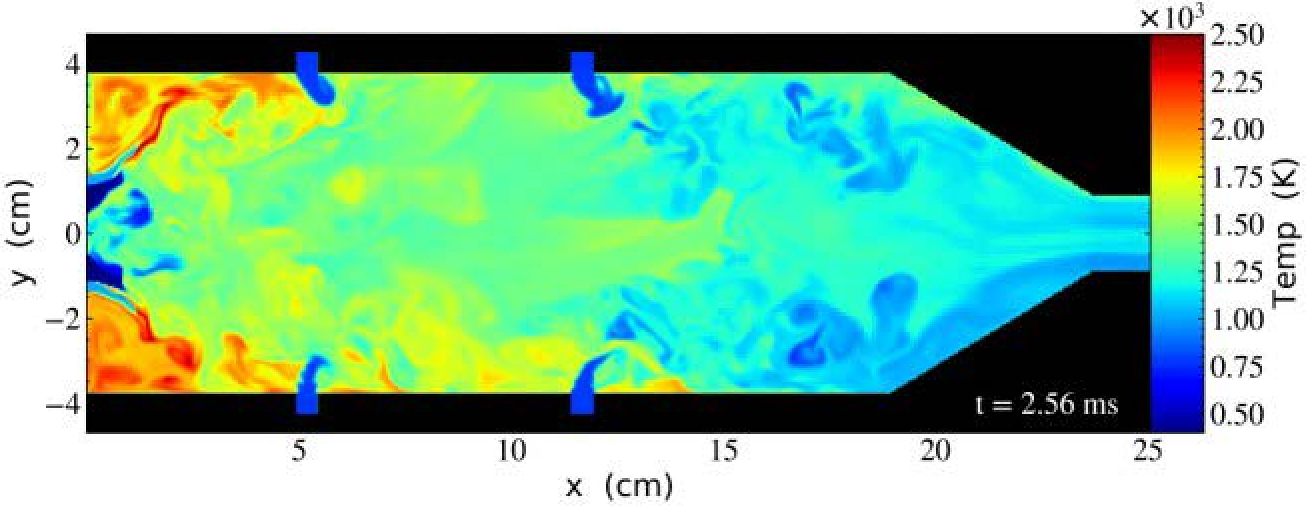
A video of our simulation is submitted to the Gallery of Fluid Motion competition.



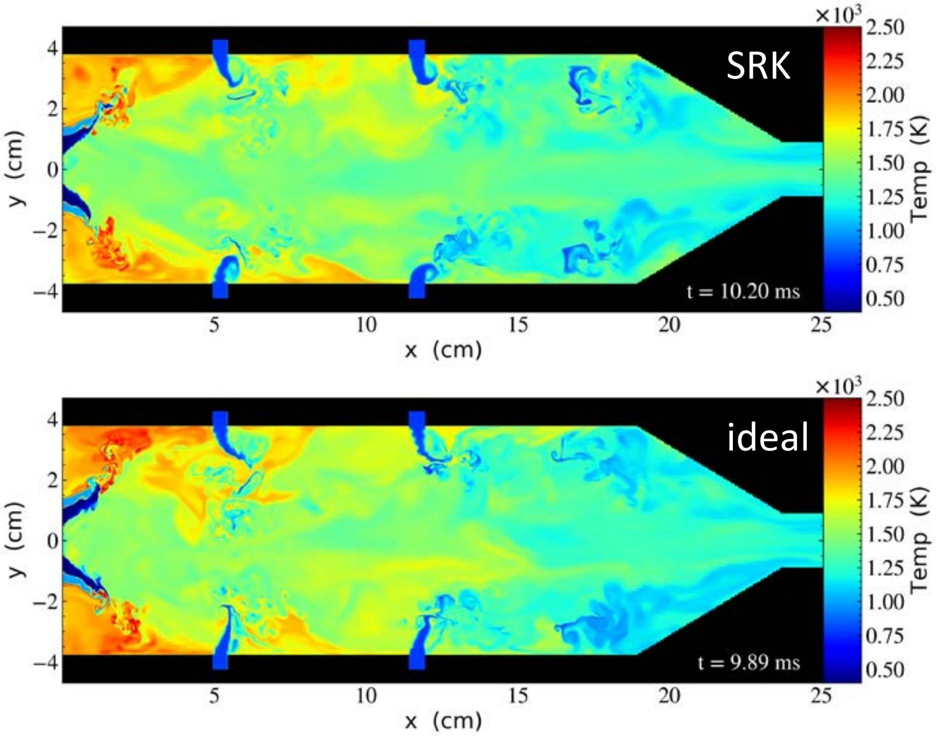
Temperature field for 100% CH_4 jet (SRK)



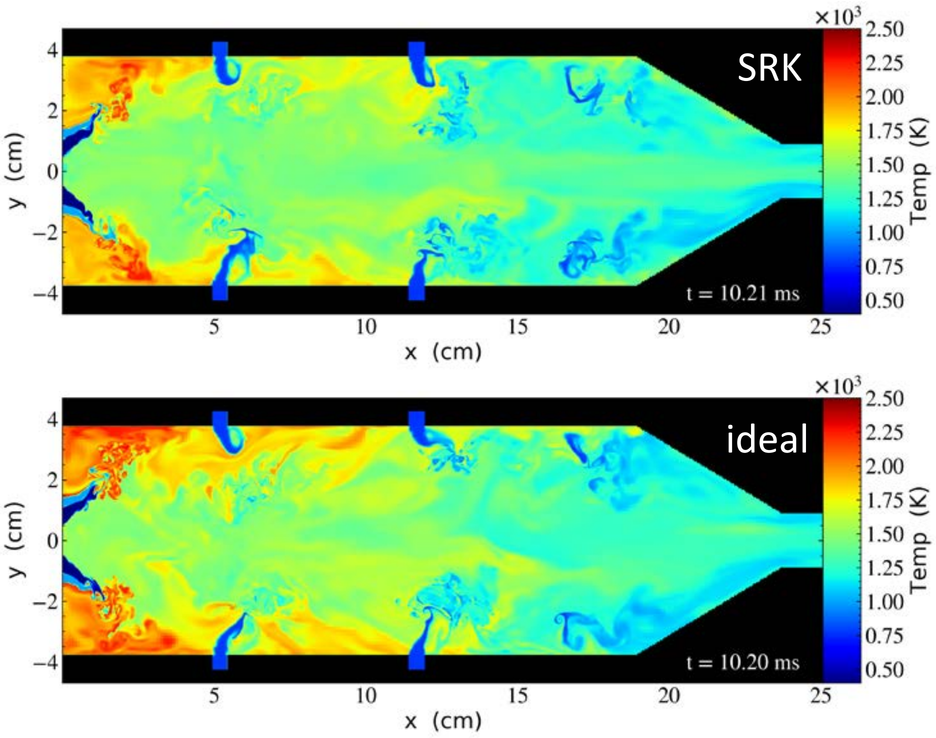
Temperature field for 100% CH_4 jet (ideal)



Impact of EOS on Temperature field

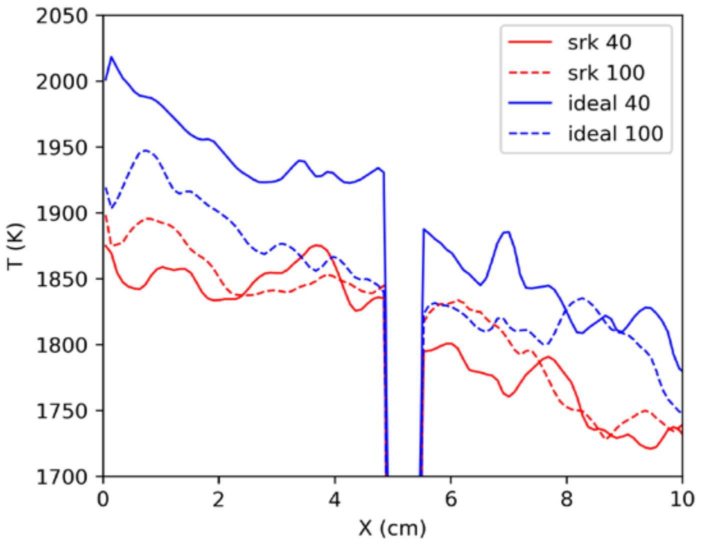


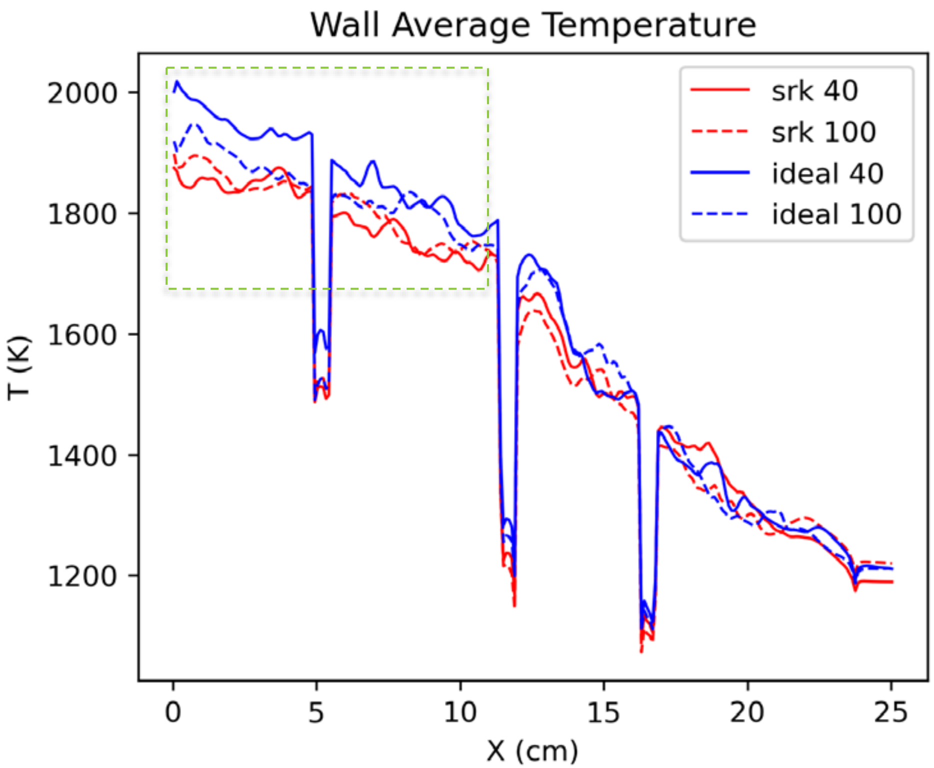
100% CH_4 jet



40% CH_4 jet

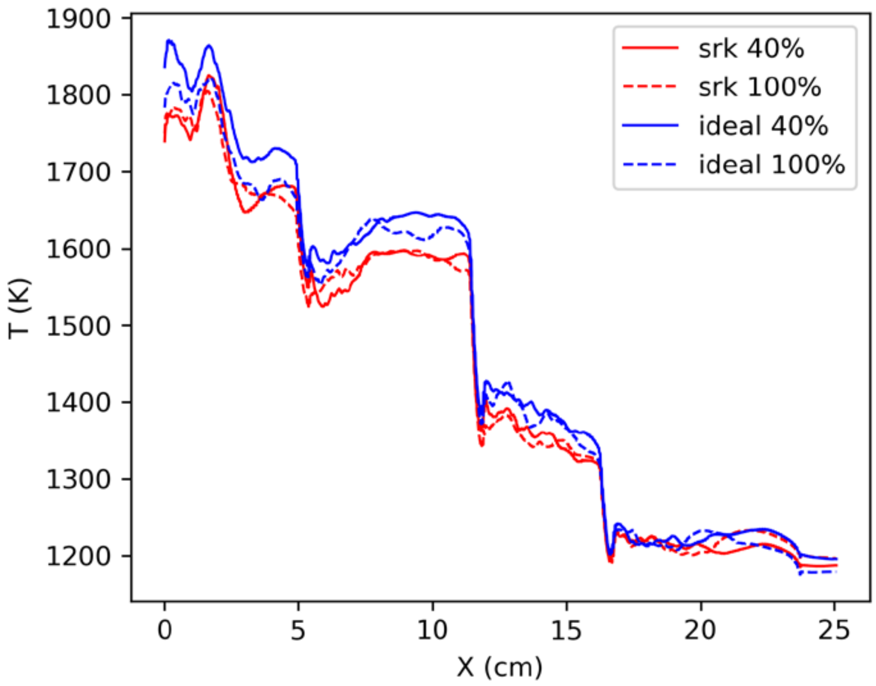
Combustor Wall Temperature

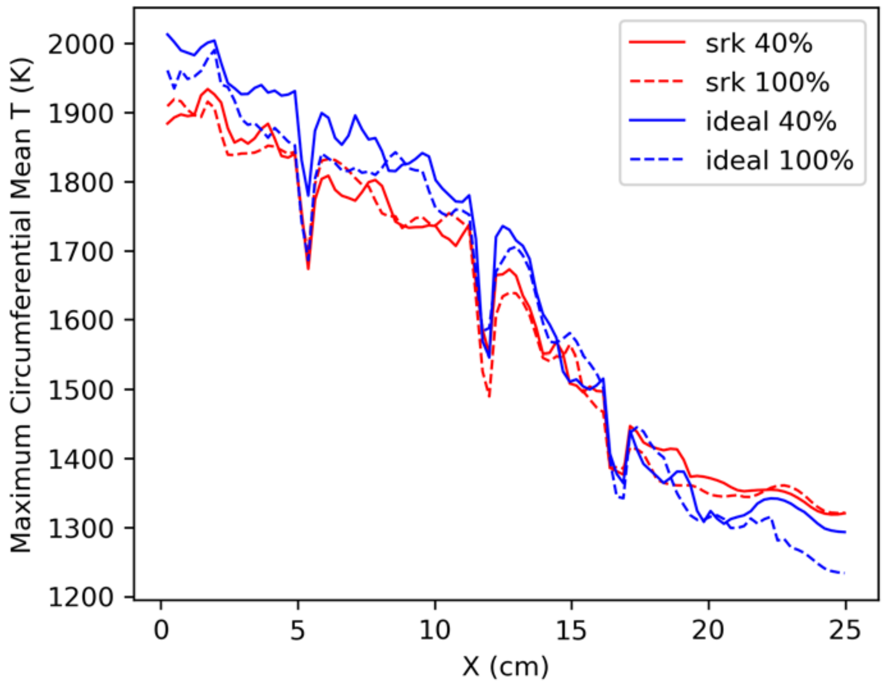




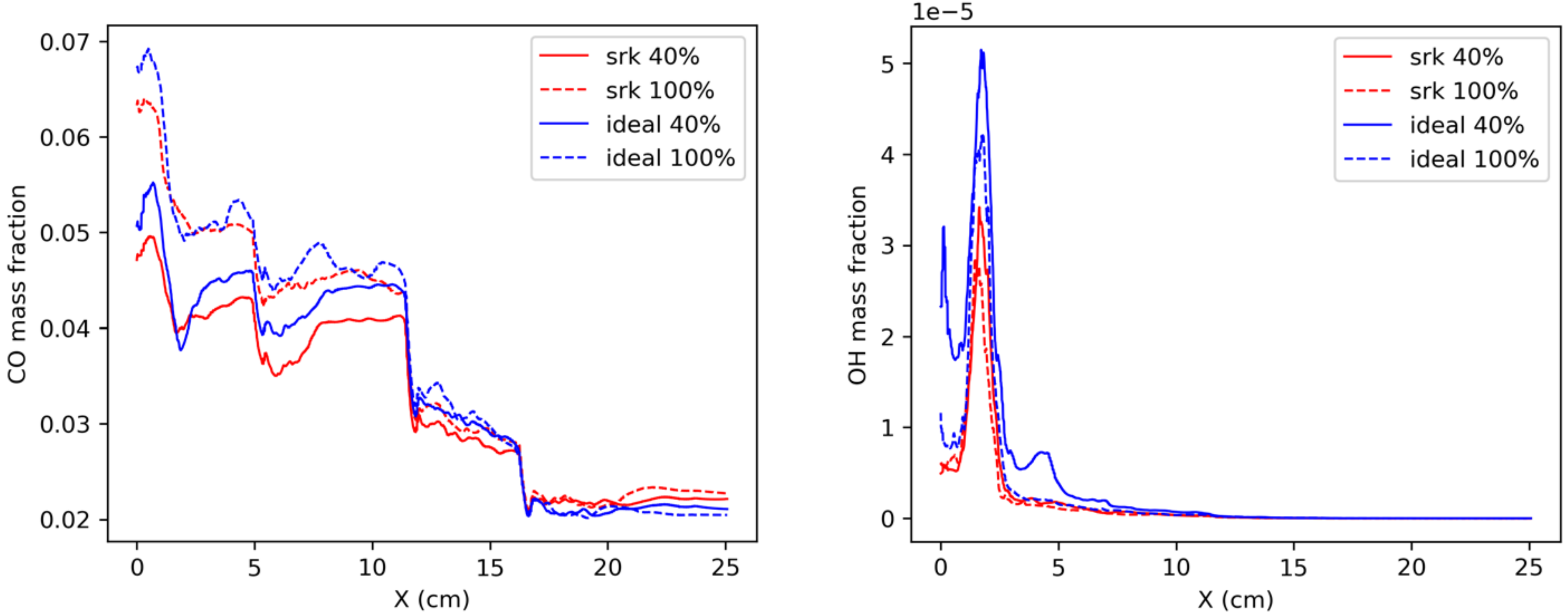
- Difference of more than 100 K for the average wall T

Axial cross-sectional average Temperature

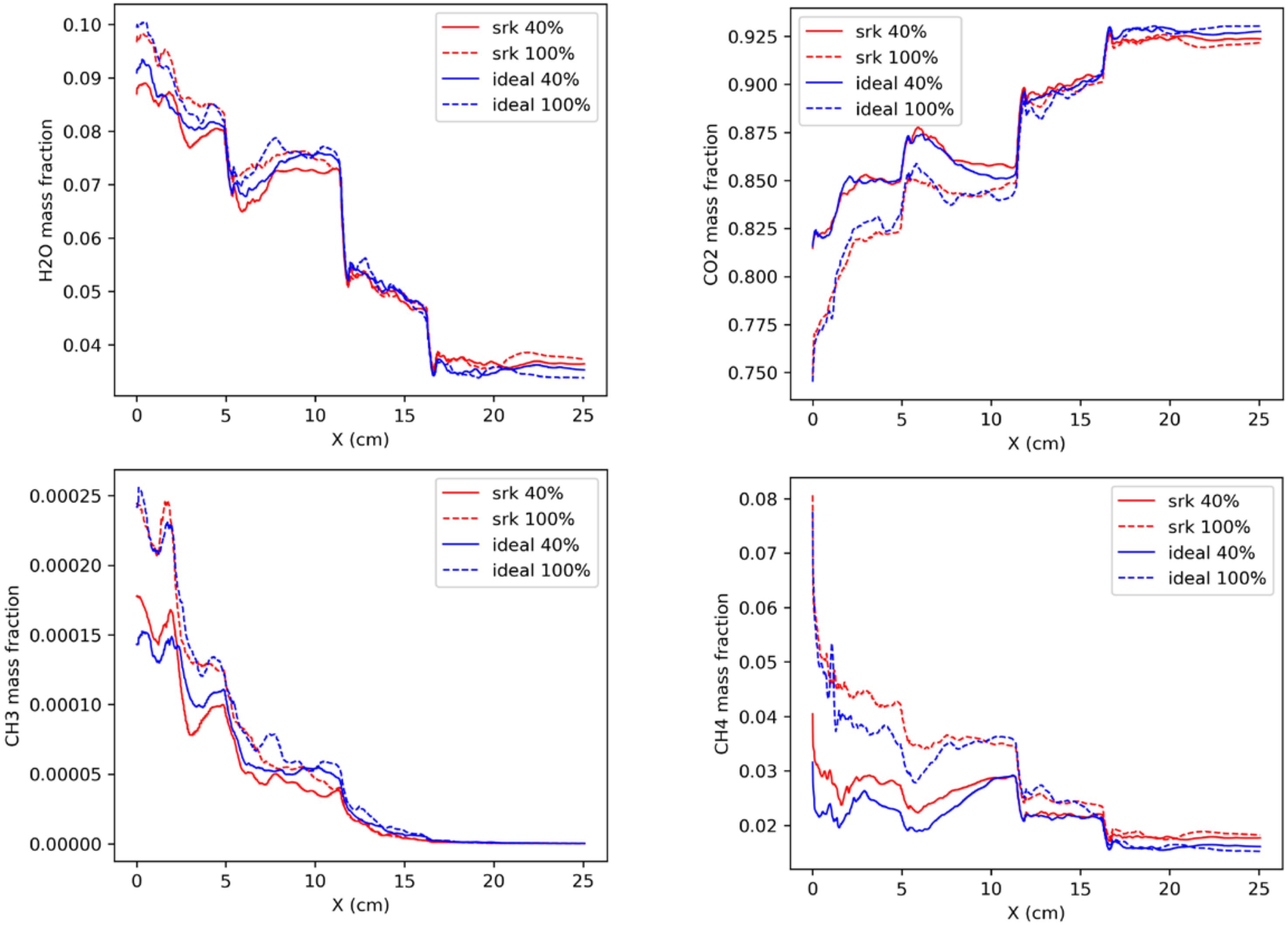




Axial cross-sectional average Species



CO formation is an important factor for the emission and safety of the combustor design


H2O mass fraction
X (cm)
CO2 mass fraction
X (cm)
CH3 mass fraction
X (cm)
CH4 mass fraction
X (cm)
srk 40%
srk 100%
ideal 40%
ideal 100%

Conclusions & Future Work

- We simulated a combustor in supercritical T, P with 2 different EOS.
- EOS impact on the flow structure, temperature, and chemistry is noticeable.
- At high T and P, choosing proper EOS is important to capture the reacting flow conditions inside the combustor (e.g. CO formation).
- Even the combustor wall temperature which is important for the design team, experience different values between the ideal and SRK EOS.

- We will further investigate this combustor with other fuel mixtures and for longer flow times.

Acknowledgements

Funding provided by U.S. Department of Energy High Performance Computing for Energy Innovation (HPC4EI) program.

Computational Resources:

- EERE HPC at NREL (Eagle)
- Office of Science HPC at ORNL (Summit)

Entry: V0074

Lighting a Match in a Fire Extinguisher
Oxycombustion in a Supercritical Carbon Dioxide Turbine

Mohammad J. Rahimi[1], Marc T. Henry de Frahan[1],
Nicholas Brunhart-Lupo[1], Bruce A. Perry[1],
Olga Doronina[1], Shashank Yellapantula[1],
Ian Cormier[2], Marc Day[1], Michael James Martin[1]

1. National Renewable Energy Laboratory
2. 8 Rivers, LLC

Thank you!

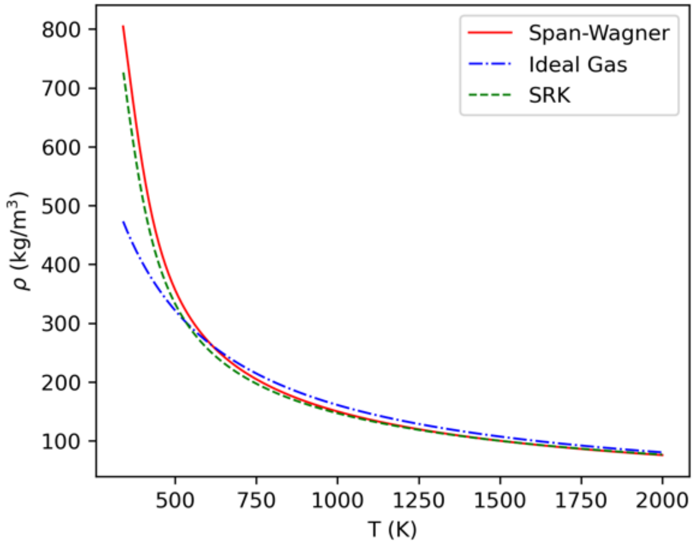
NREL/PR-2C00-88165

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Bioenergy Technologies Office. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

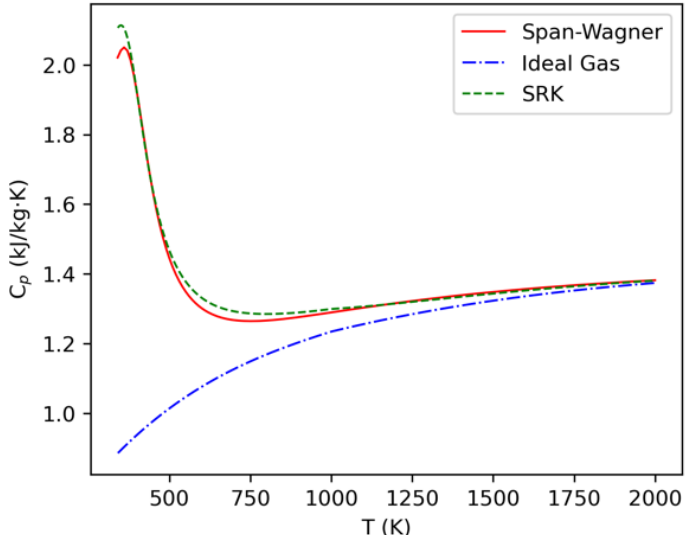
NREL Transforming ENERGY

Extra

Choice of equation of state a balance of accuracy, computational efficiency.



Density vs. temperature at 303.9 bar



Specific heat vs. temperature at 303.9 bar

AMR capturing areas of most interest in flow