High-fidelity simulations of supercritical CO_2 based oxy-combustion with non-ideal equation of state

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Power cycle

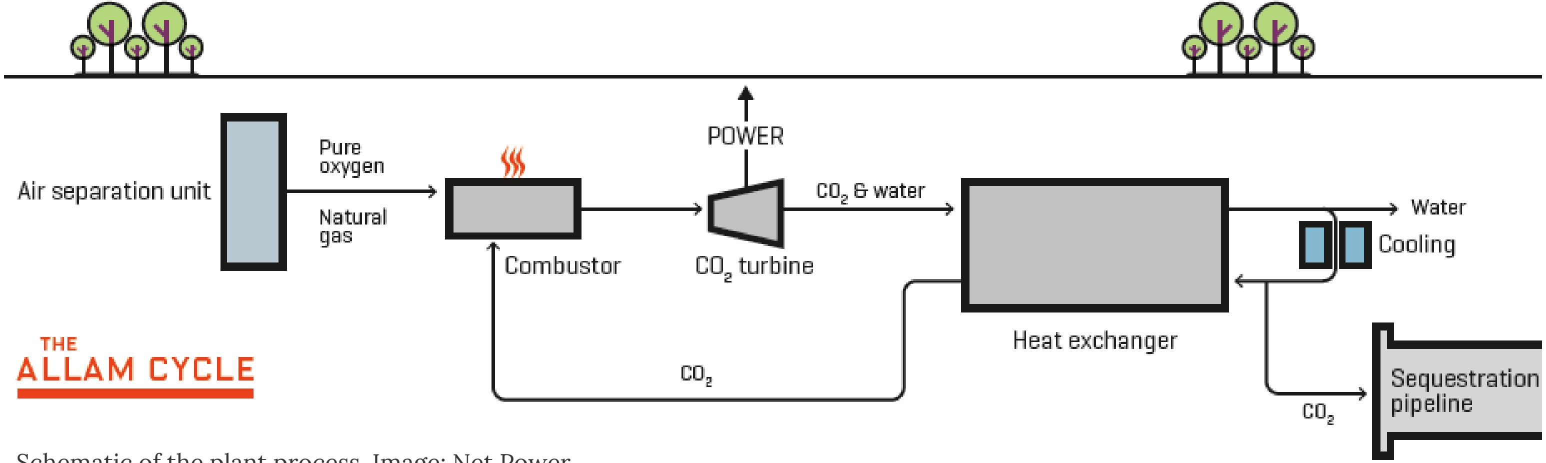
Capture ~100% of atmospheric emission

High-temperature oxy-combustion of carbon fuels

- Oxygen is used instead of air, eliminating NO_x emissions

High-pressure sCO2 as working fluid (T_c = 304.13 K, P_c = 73.8 bar)

- Produced CO2 can be recirculated within the same cycle loop
- The excess CO2 from the cycle can be used for other commercial purposes

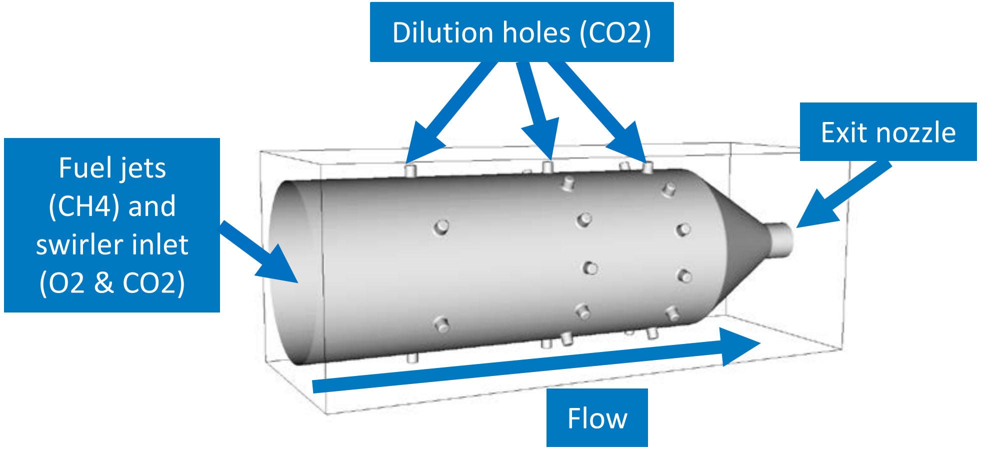


Schematic of the plant process. Image: Net Power

sCO2 based oxy-combustor

sCO2 combustor operating conditions

- 200–300 bar pressure
- 800–1000 K inlet temperature
- The percentage of sCO2 should be more than 95% by mass



Modeling challenges:

- Small scale turbulence
- Complex multi-inlet geometry
- Complex chemical kinetics
- Existing models were developed for lower $T,\ p,\ Y(\mathrm{CO_2})$

2D case set up

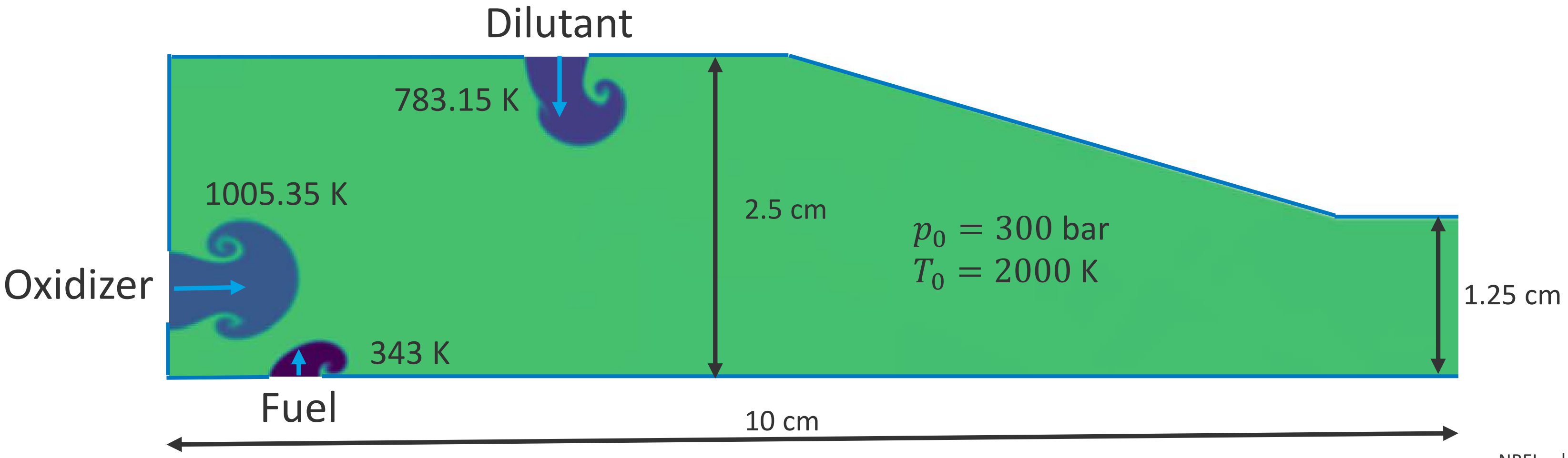
		T [K]	d [cm]	$\dot{m}$ [g/s]
Fuel	CH_4	343.15	0.4	101.2
Oxidizer	$0.8CO_2 + 0.2O_2$	1005.35	0.6	449.75
Dilutant	CO_2	783.15	0.5	337.32

Momentum ratio

$$\frac{\rho_{ox} U_{ox}}{\rho_f U_f} = \frac{\dot{m}_{ox} d_f}{\dot{m}_f d_{ox}} = 4$$

Equivalence ratio

$$\phi = \frac{1}{(F/O)_{st}} \frac{\dot{m}_f}{\dot{m}_{ox}} = 0.9$$



PeleC

PeleC

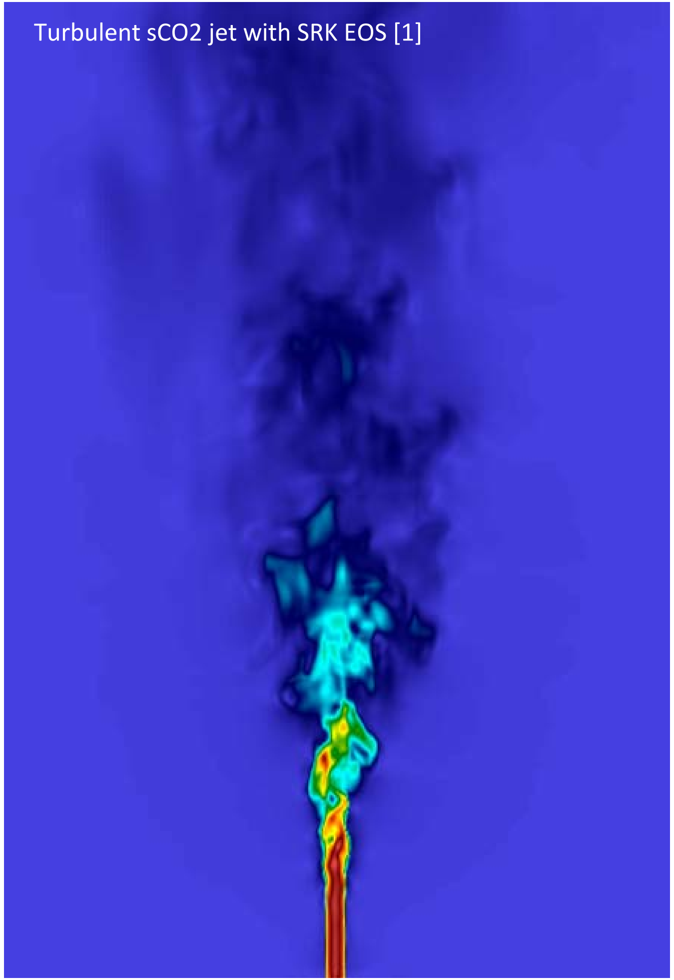
- Finite volume compressible solver
- for reacting flow

AMReX

- Adaptive mesh refinement (AMR)

PelePhysics:

- Models and parameters for thermodynamics
- Transport properties (viscosity, etc)
- Chemical reactions and finite rate chemistry integration (SUNDIALS)
- EOS: ideal gas mixtures and Soave-Redlich-Kwong (SRK)


Turbulent sCO2 jet with SRK EOS [1]

Equation of State

Operating pressure 300 bar

- The supercritical condition for many of the reactants and products
- Intermolecular forces are not negligible
- The ideal gas assumption is not valid

Ideal gas EoS

$$p = R_u T \sum \frac{Y_k}{W_k} \frac{1}{v}$$

Assumptions:

- Negligible volume of particles
- No intermolecular forces
- Perfect elastic collisions with no energy loss

Soave-Redlich-Kwong (SRK) EoS

$$p = R_u T \sum \frac{Y_k}{W_k} \frac{1}{v - b_m} - \frac{a_m}{v(v + b_m)}$$

$$a_m = a_m(T, Y_k) = \sum_{ij} Y_i Y_j \alpha_i \alpha_j \, ; \quad b_m = b_m(Y_k) = \sum_k Y_k b_k$$

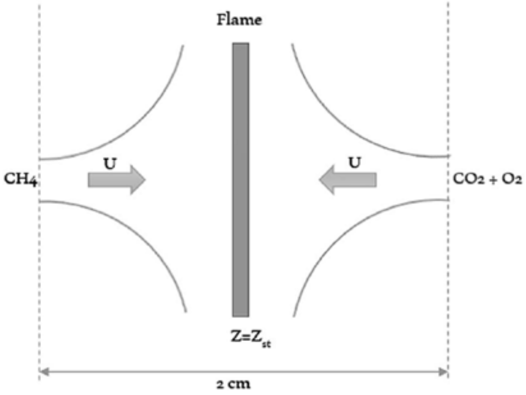
Accounts for:

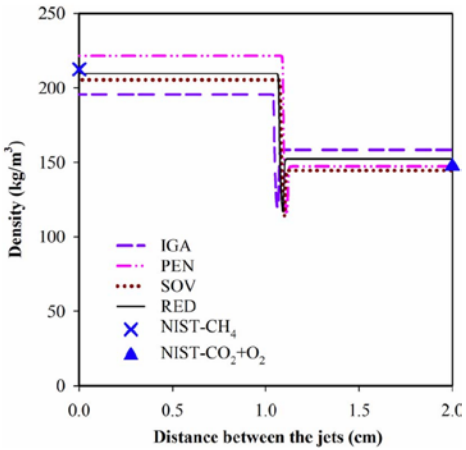
- Finite molecular dimensions
- Interactions between the molecules

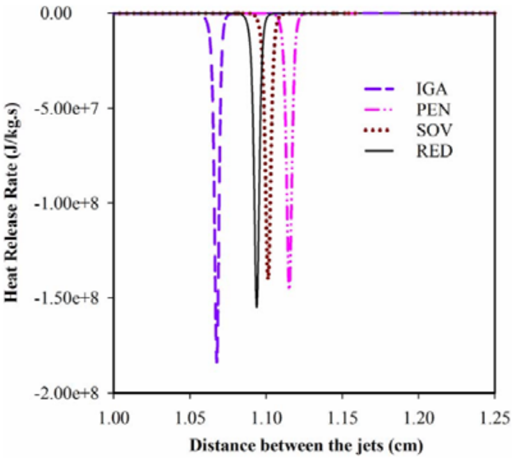
Influence of EoS

[1] K.R.V. Manikantachari et al (2020).

- Simulating counter-flow sCO2 flames
- $P = 300\ \text{atm},\ T_{ox} = 1000\ \text{K},\ T_f = 300\ \text{K},\ Y_{CO_2}\ \text{in oxidizer} = 0.96$
- Non-ideal effects are significant for fuel jets. ~12% difference in density
- Choice of EoS significantly influences momentum of jets, flame structure, het release rate, etc.

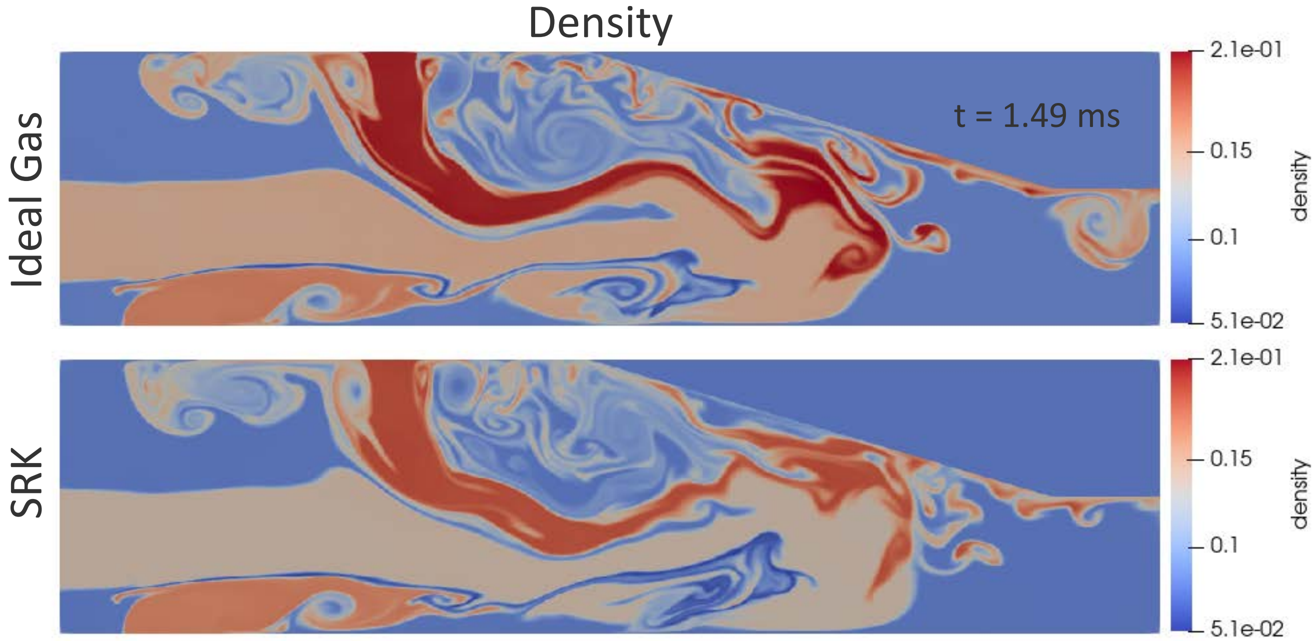






Preliminary results

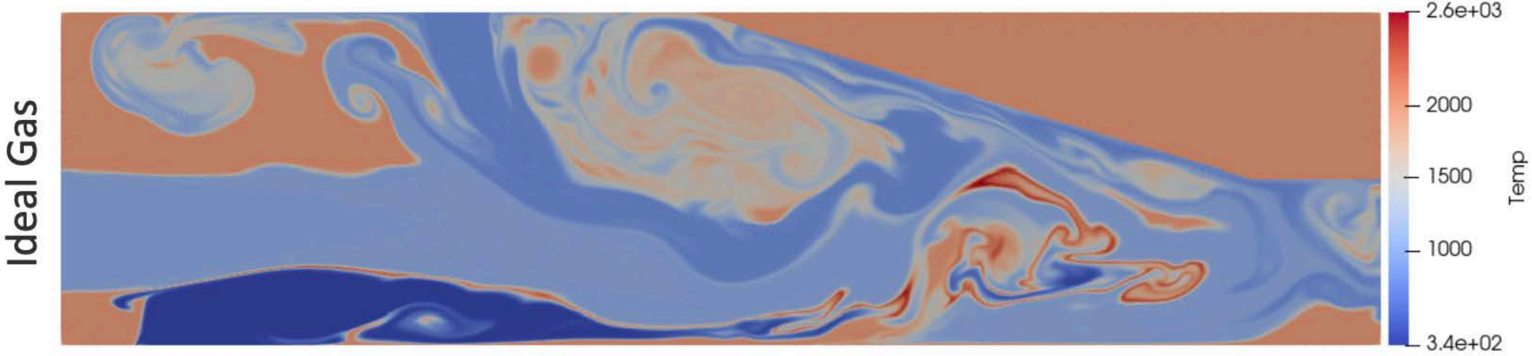
CFL = 0.2, Mesh 1024x256



The EOS is a crucial model for density estimation in a simulation.

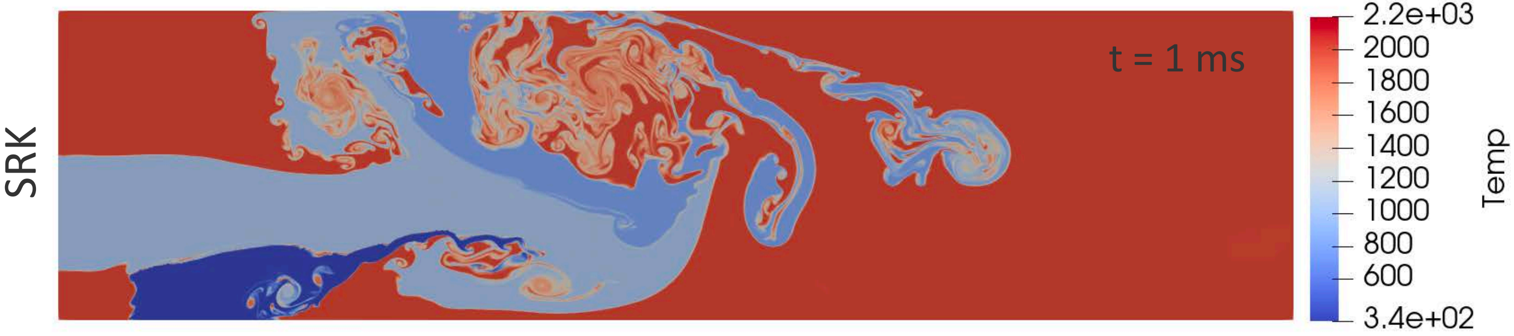
Preliminary results

- Flame burns at oxygen-CH4 interface
- Streams interacts with turbulence
- Forms recirculation areas


Temperature

Future plans

- **Higher resolution runs**
    - 2048x512 + 3 level AMR (0.61e-5 m)
    - Different % of CH4 in the fuel
    - Exit plane analysis



Questions?

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