Design and Modeling of an 80 bar Oxy-Combustor for Direct Fired Supercritical CO_2 Power Generation

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Outline

- Background and Motivation
- Oxy-Combustion Fundamentals and Validation Modeling Examples
- Experimental Layout
- Operating Conditions
- CFD Setup and Results

Motivation

Direct-Fired sCO_2 Cycles

- Direct-fired (Allam) cycle operates at very high pressures (300 bar) with CO_2 dilution.
- CFD is expected to play a key role in combustor design (flame holding, heat release, CO formation, etc…).
- There is a lack of experimental data and modeling experience at these conditions.

Approach – Develop experimental capability at relevant conditions and validate computational tools.

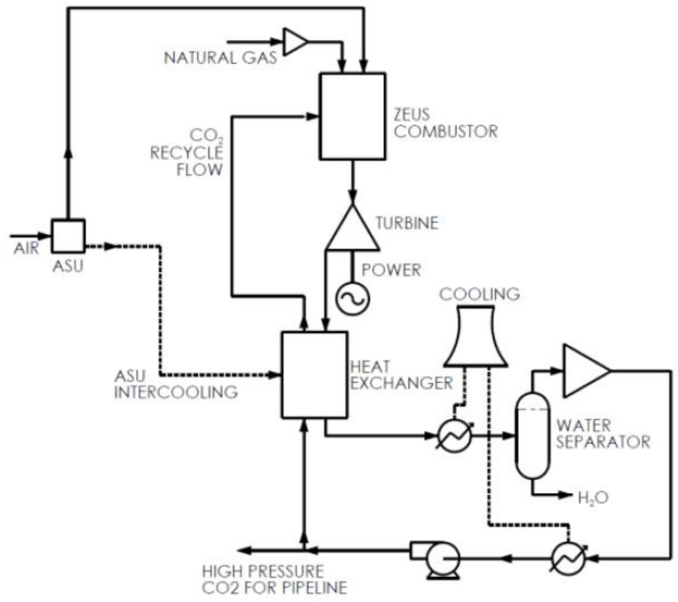


Table 1. ALLAM CYCLE KEY POINTS (ISO CONDITIONS)

Point	Pressure (Bar)	Temperature (°C)
Turbine Inlet (A)	300	1150
Turbine Outlet (B)	30	775
CO2 Compressor Inlet (D)	30	20
CO2 Compressor Outlet (E)	80	65
CO2 Pump Inlet (F)	80	20
CO2 Pump Outlet (G)	300	55
Combustor Inlet (I)	300	750

** Allam, et al., Energy Procedia 37, 2013, 1135-1149*

Borghi Diagram for Oxy-Combustion

- **Three cases shown for 300 bar oxy-combustion define a range of conditions (O_2 mass fraction from 7-25%) spanning the thickened, corrugated flame regime and stirred reactor.**

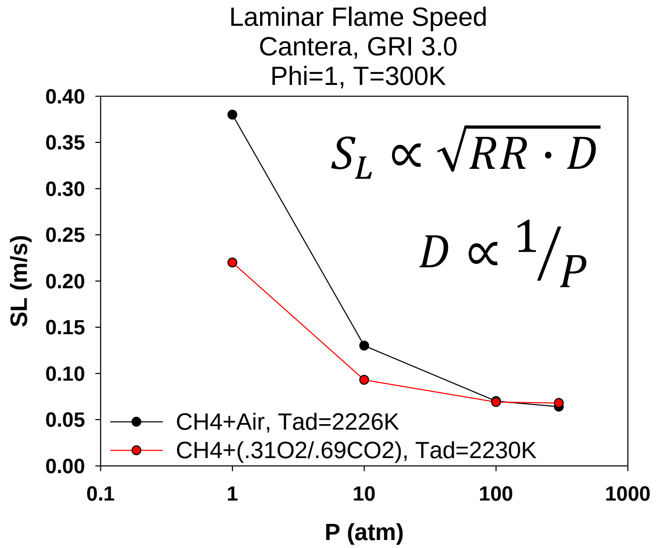
$$Ka = \frac{\tau_{chem}}{\tau_K} = \frac{\delta_L^2}{l_K^2}$$

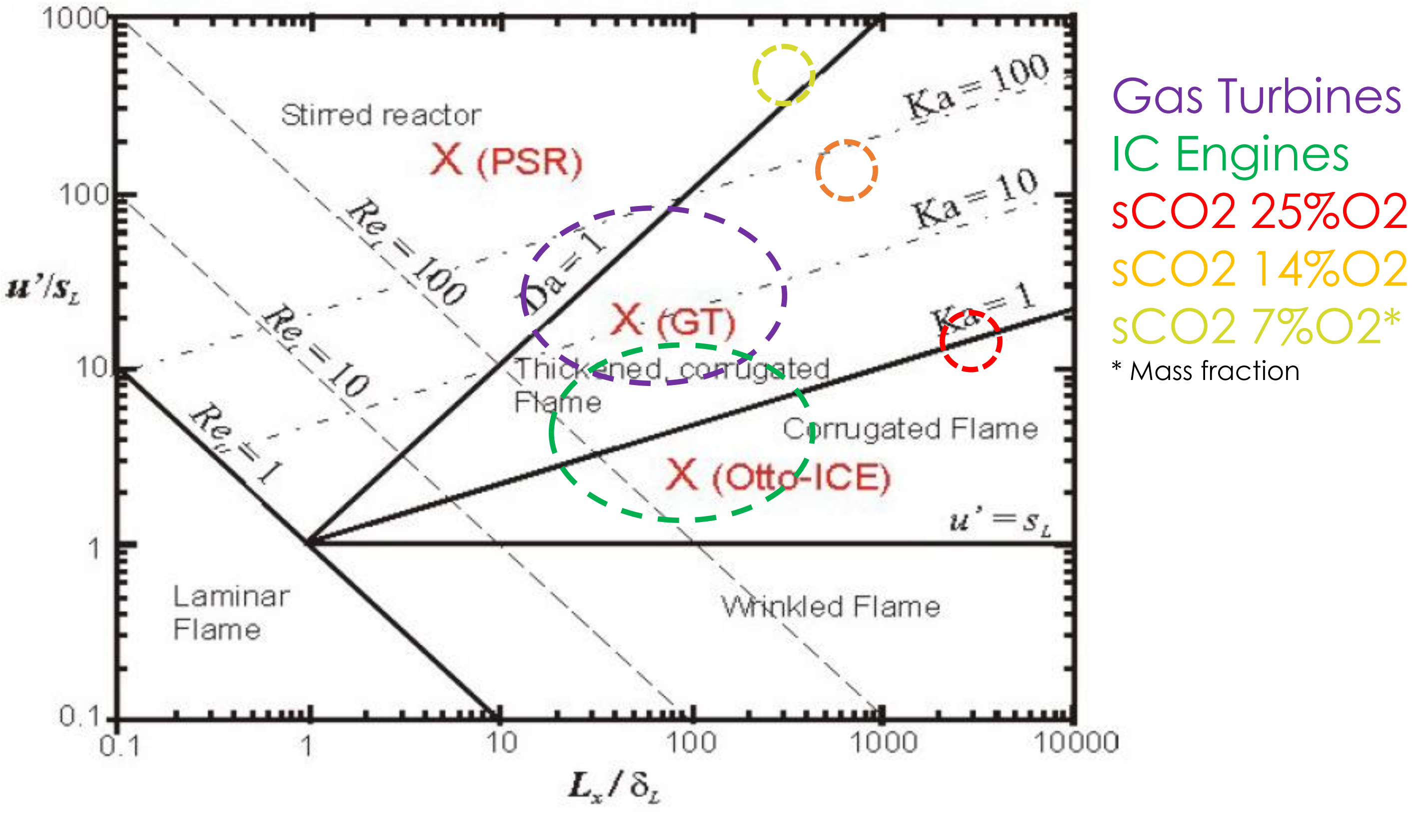
- **Significantly outside the range of gas turbine and IC engine operation.**
- **Requires assessment of appropriate turbulent combustion models.**

Laminar Flame Thickness

$$\delta_L = \frac{\alpha}{S_L}$$

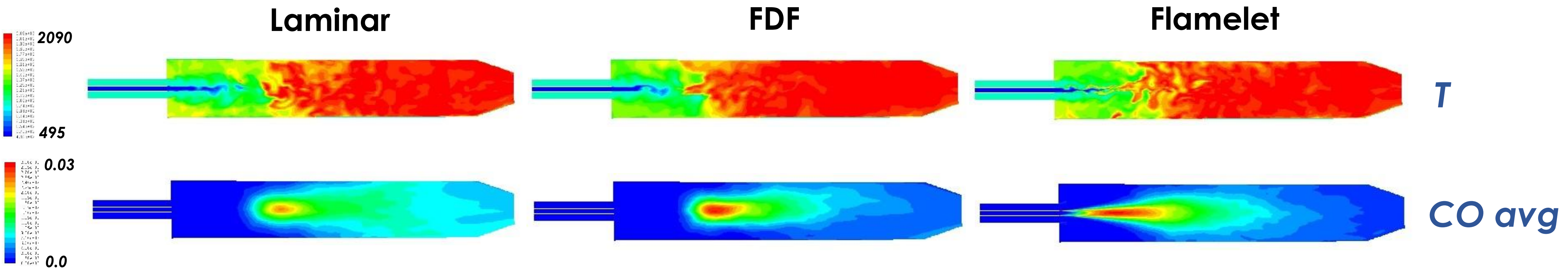
$$\alpha = k/\rho C_P$$



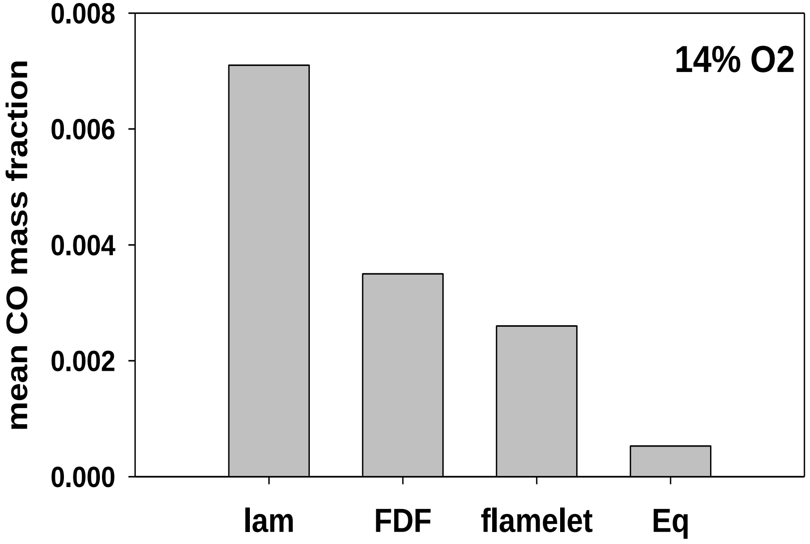


Example of Three TCI Models

LES Comparison of FDF, Flamelet and No Model



- Significant differences in predicted CO mean mass fraction at the combustor exit.
- Need to validate!

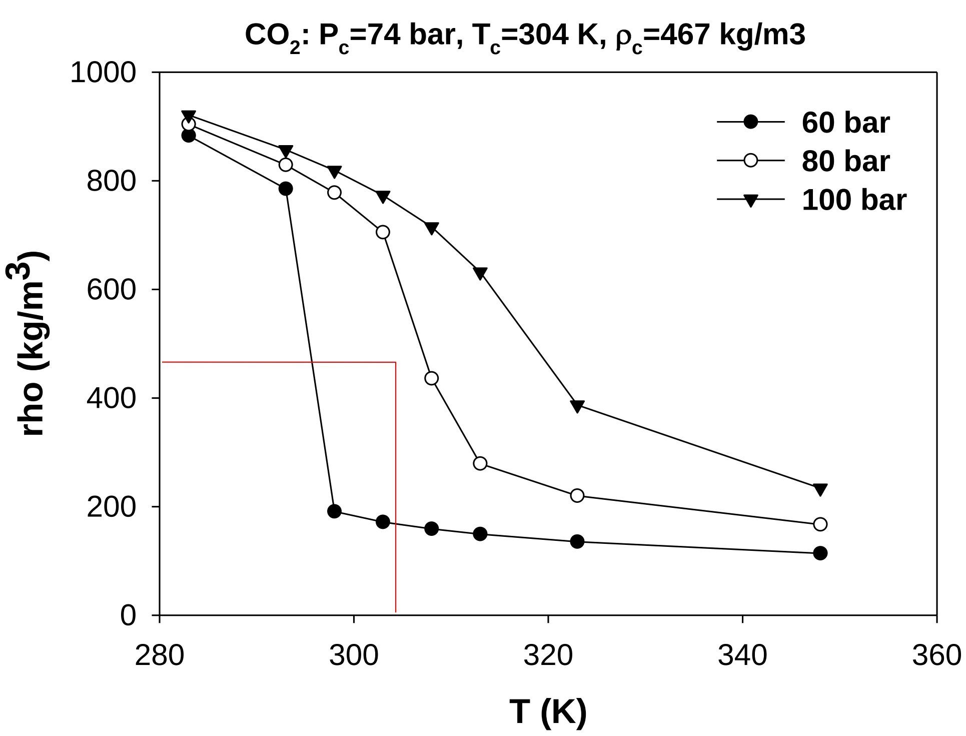


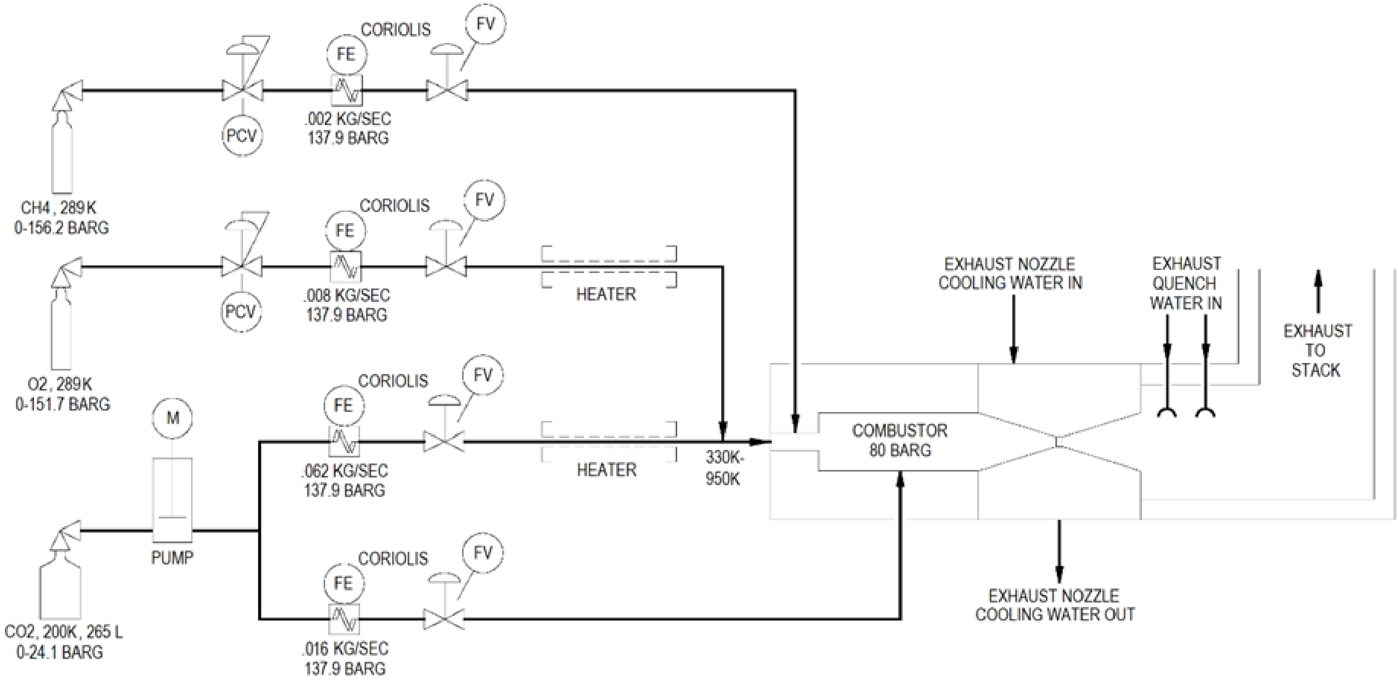
Phi = 0.95
T_F = 476 K
T_O = 1014 K
P = 300 bar
2.4 MW

- *LES, 16 Species skeletal mechanism from UCF*
- *ANSYS Fluent V18.2*

Experimental Layout and CO_2 Properties

80 bar Max Combustor Pressure

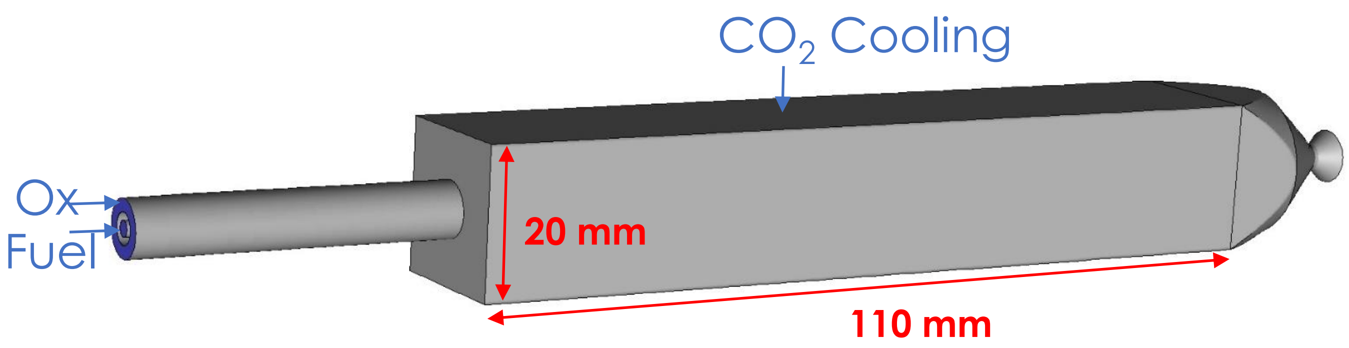




- 80 bar chosen as a compromise between cost and relevancy.
- Blow-down from standard k-bottles for CH_4 and O_2
- CO_2 from liquid dewar with pump and heater (330K initially, 950K later).

Experimental Layout and Operating Conditions

80 Bar Optically Accessible Combustor



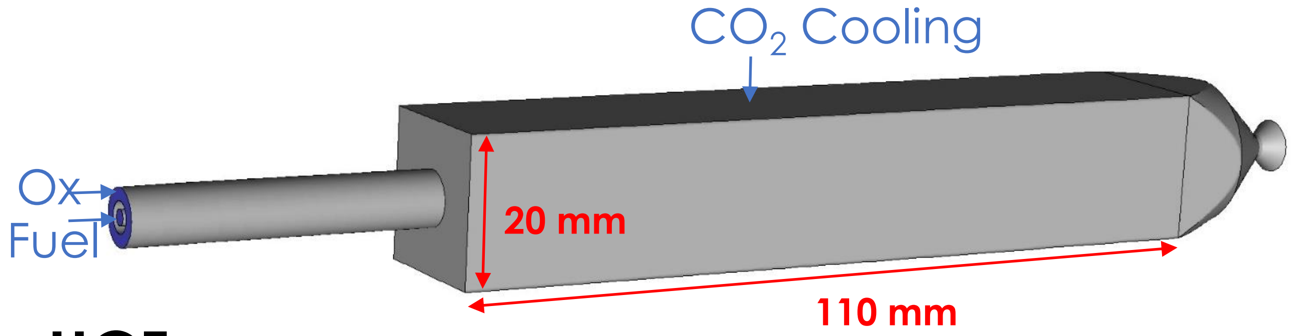
	Case 1	Case 2	Case 3	Case 4
O_2 Mass Fraction in Oxidizer	0.3	0.3	0.3	0.3
Heat Input (kW)	100	100	25	25
Fuel Flow (g/s)	2.0	2.0	0.5	0.5
Oxidizer Flow (g/s)	26.68	26.68	6.67	6.67
U_{ox} (m/s)	21.4	7.4	5.3	1.9
Re_{ox}	34,700	85,200	8,670	21,300
U_{fuel} (m/s)	11.4	11.4	2.8	2.8
Re_{fuel}	64,600	64,600	16,100	16,100
T_{ox} (K)	950	330	950	330
Mom flux (ox/fuel)	2.82	0.98	2.82	0.98
CO_2 cooling (g/s)	40.0	40.0	40.0	40.0

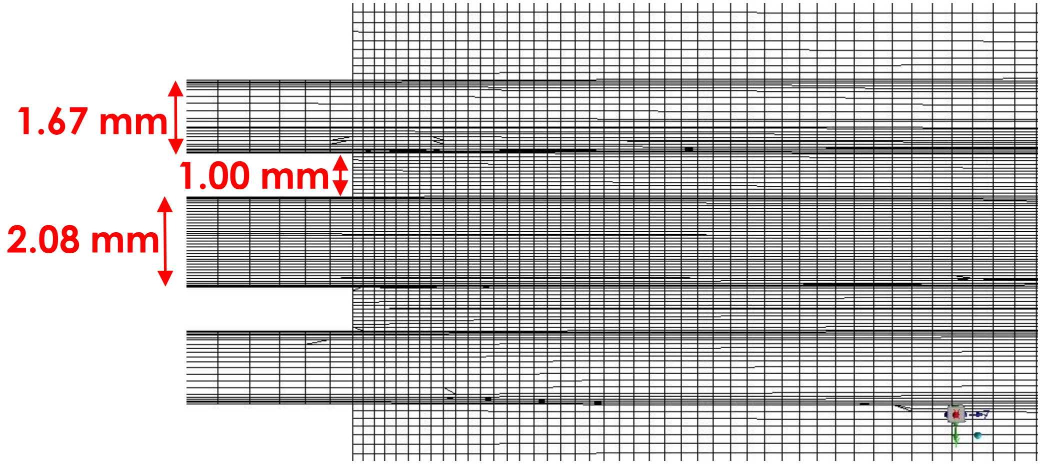
- **Two flow rates (100 and 25 kW).**
- **Two oxidizer preheat temperatures (330K and 950K).**
- **Transpiration and backside water cooling.**

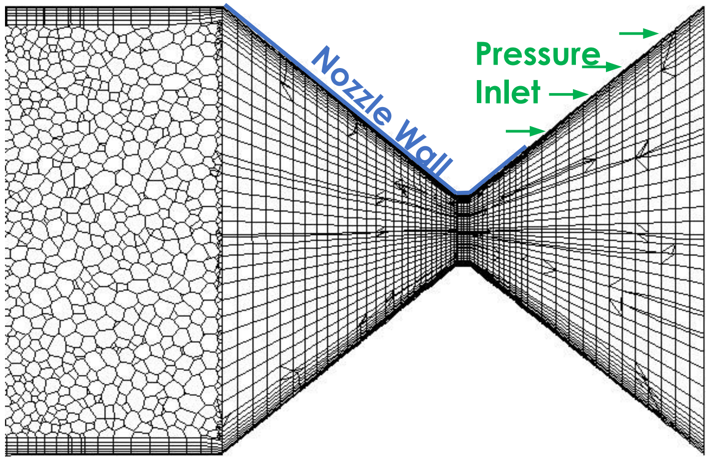
Combustor Design and Modeling Setup

3D LES and RANS with Skeletal Chemistry

- 1.7M cells.
- No nozzle on most simulations.
- ANSYS Fluent 22.1.
- 16 species skeletal mechanism from UCF.
- RANS realizable k-e or LES with transported k.
- 2nd order.

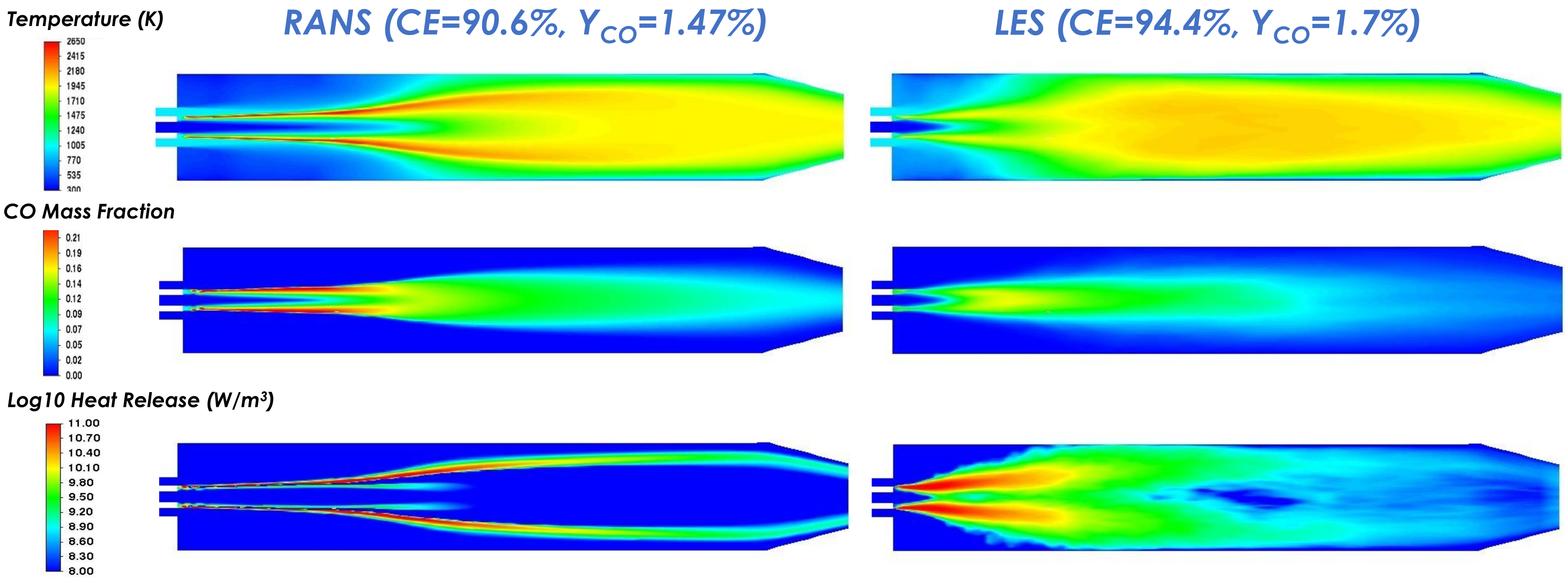






Results for Case 1 (baseline)

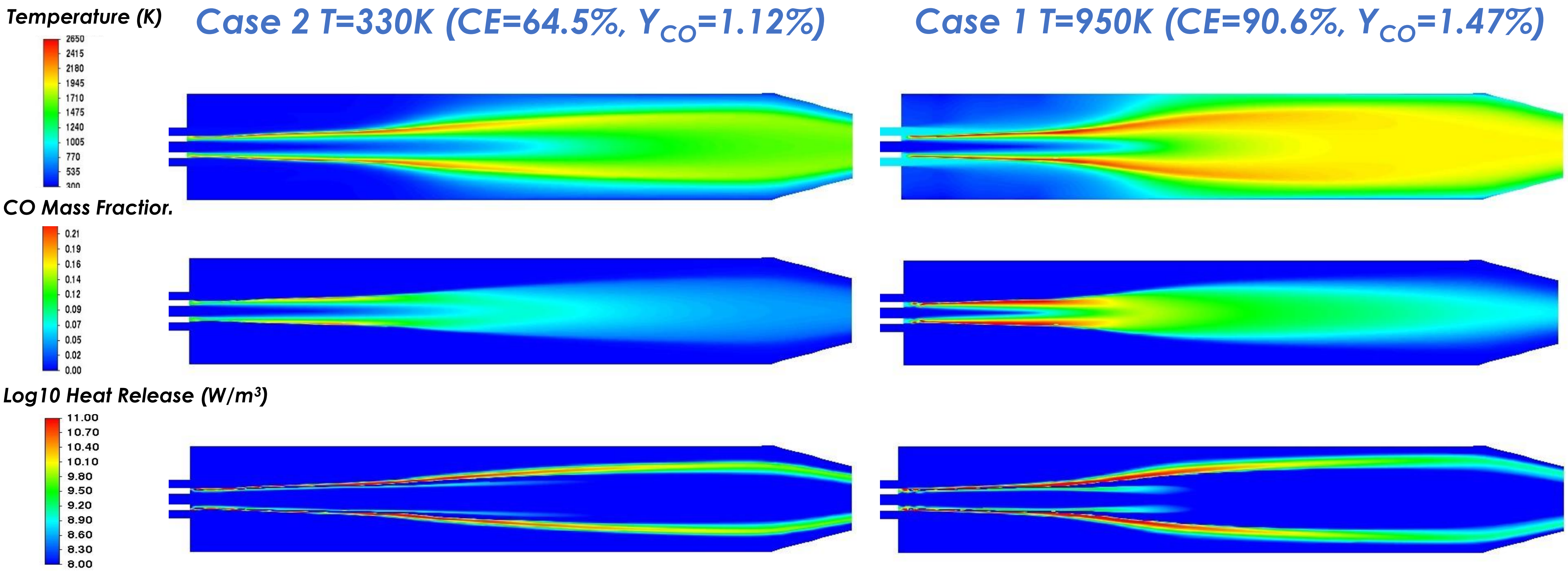
Case 1: 100 kW, T=950K preheat



- RANS predicts long flame, LES predicts shorter flame (faster mixing).
- No unburned CH_4 but significant CO emissions.

Effect of Oxidizer Preheat Temperature

RANS: 100 kW



- Lower preheat temperature results in slower kinetics and 27% of CH_4 exiting combustor unburned.
- Non-reacting simulations show slower mixing with lower preheat temperature due to lower ox-to-fuel momentum ratio.

Effect of Flowrate at Lower Preheat Temp

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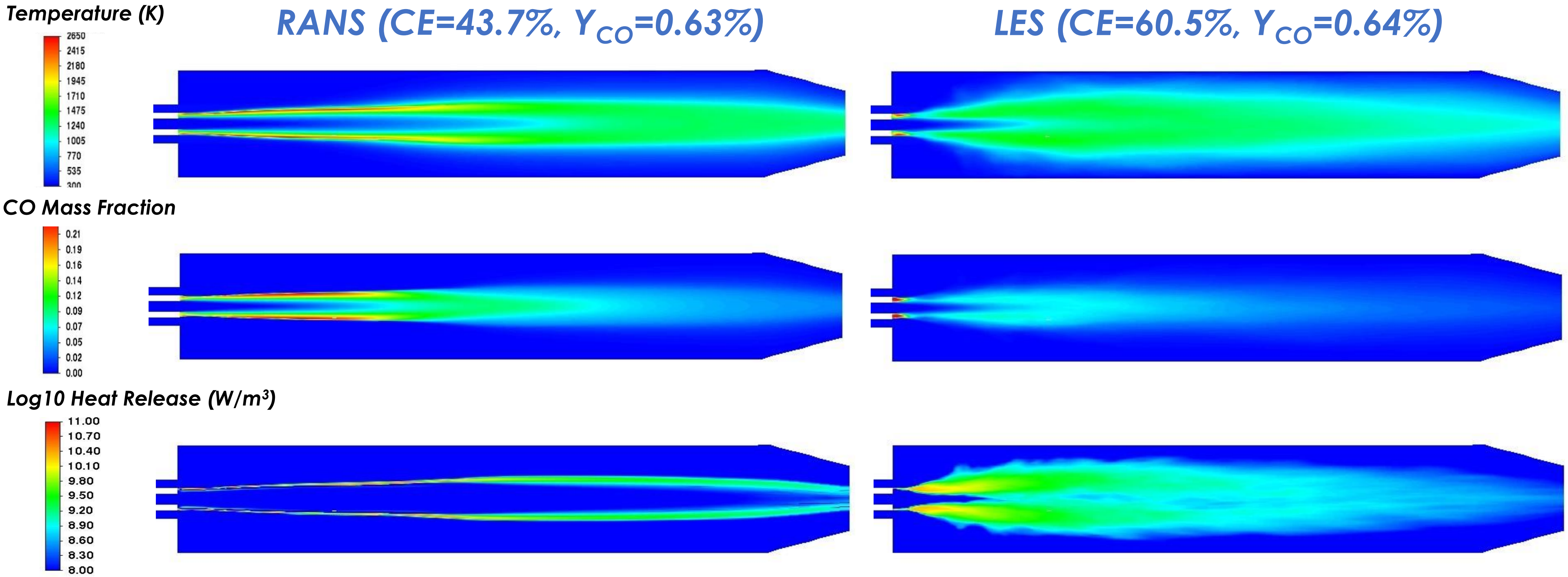
Case 4: 25 kW, T=330K Preheat

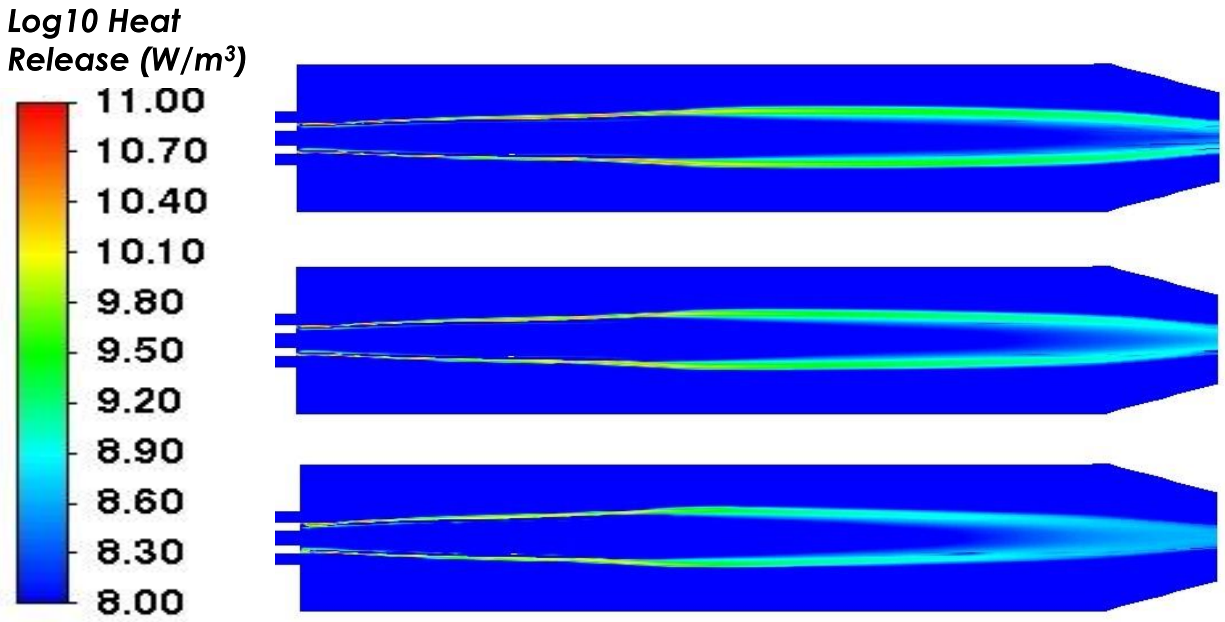


- **RANS predicts a significantly longer flame length and lower combustion efficiency compared to LES. Slower mixing.**
- **Large fraction of CH_4 exiting combustor unburned (43.4% for RANS case).**

Effect of Combustor Pressure

Case 4: 25 kW, T=330K Preheat

Flowrates for 60 and 40 bar cases scaled by pressure



80 bar — *CE=43.7%, Y_{CO}=0.63%, m_{ch4}=43.4%*

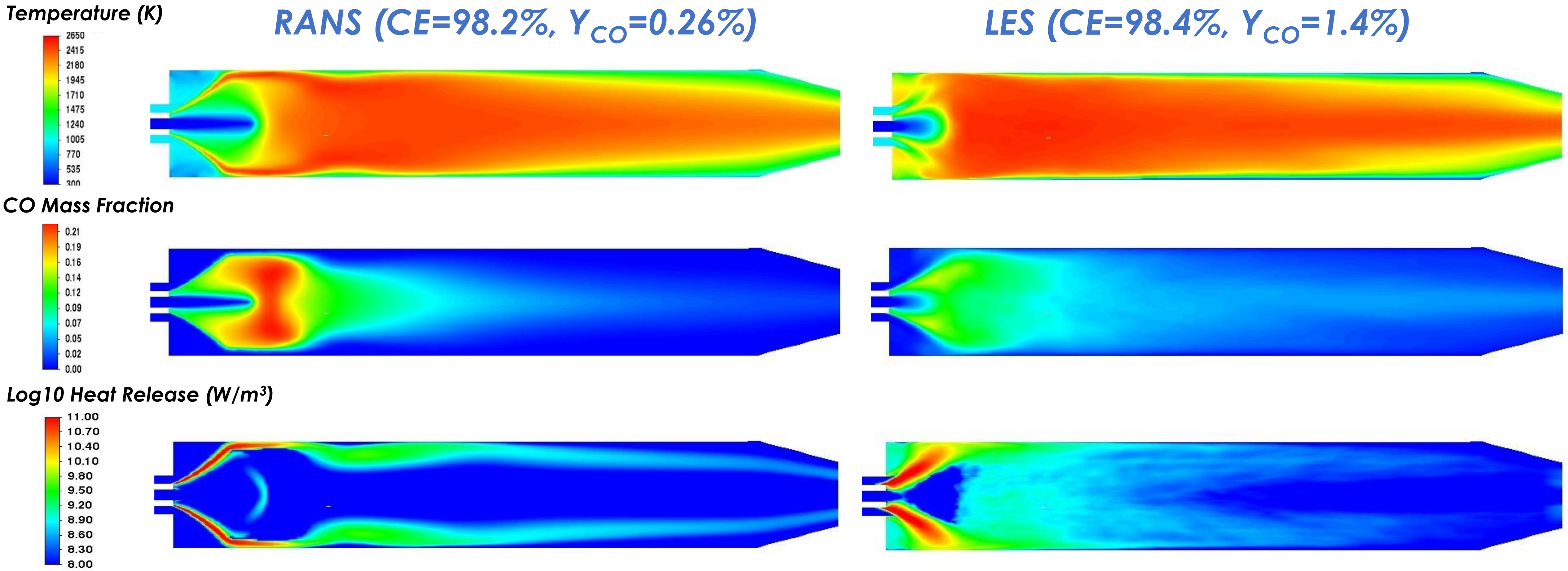
60 bar — *CE=42.6%, Y_{CO}=0.63%, m_{ch4}=44.7%*

40 bar — *CE=41.1%, Y_{CO}=0.61%, m_{ch4}=46.4%*

- Operating pressure has small effect on heat release profile.
- Combustion efficiency increased from 41.1 to 43.7% as pressure increased.

Swirling Oxidizer Flow (45°)

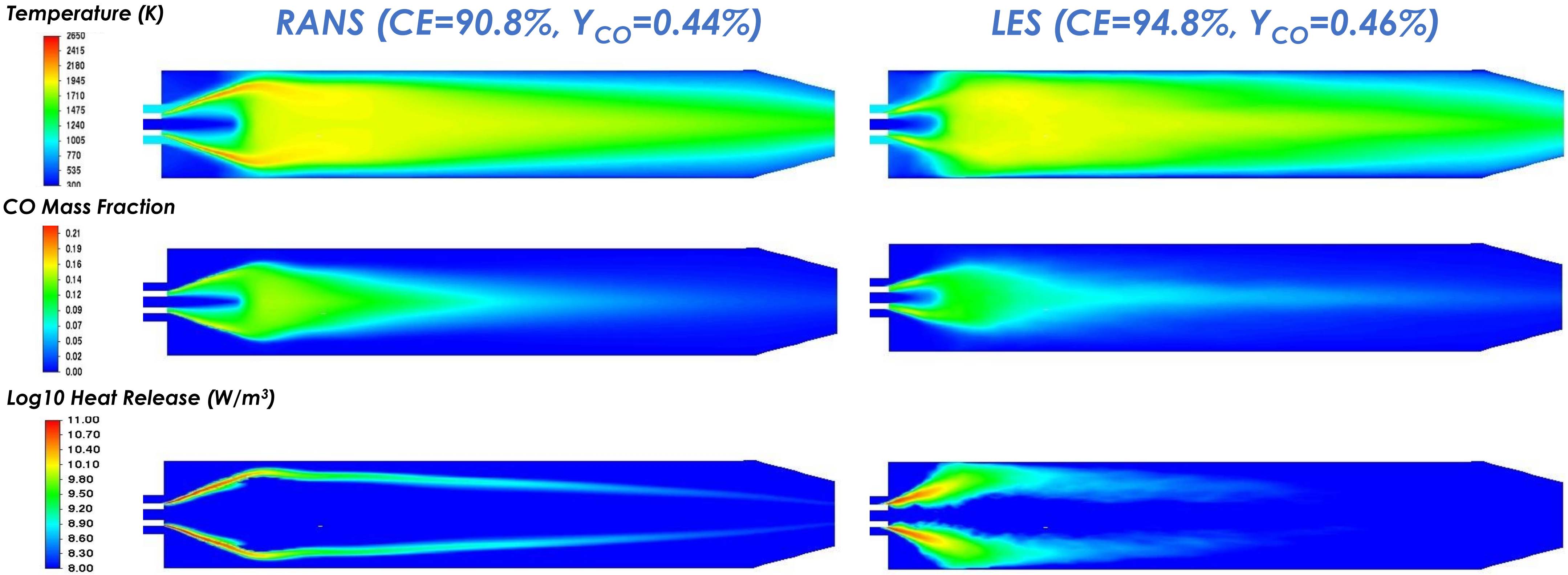
Case 1: 100 kW, T=950K preheat



- Swirl drastically reduces flame length with most of heat release occurring in first 30 mm of the combustor. Much higher combustion efficiency and lower CO as well.
- Greater similarity between RANS and LES for swirling cases.

Swirling Oxidizer Flow (45°)

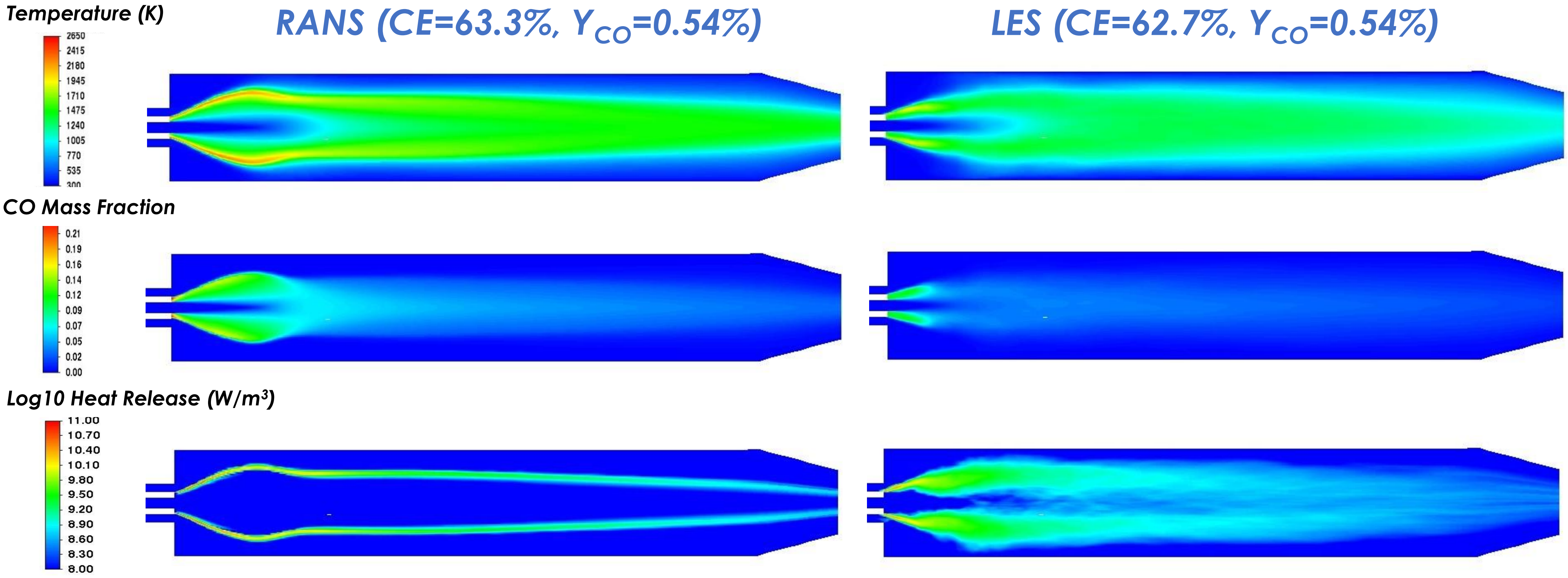
Case 3: 25 kW, T=950K Preheat



- Drop in combustion efficiency with lower preheat temperature.
- Unburned CH_4 was roughly 2.5%.

Swirling Oxidizer Flow (45°)

Case 4: 25 kW, T=330K Preheat



- Swirl improves combustion efficiency over non-swirling case (~43%).
- Unburned CH_4 was 27% for RANS and 32% for LES.
- Roughly 28% of fuel converted to CO.

Nozzle Heat Transfer

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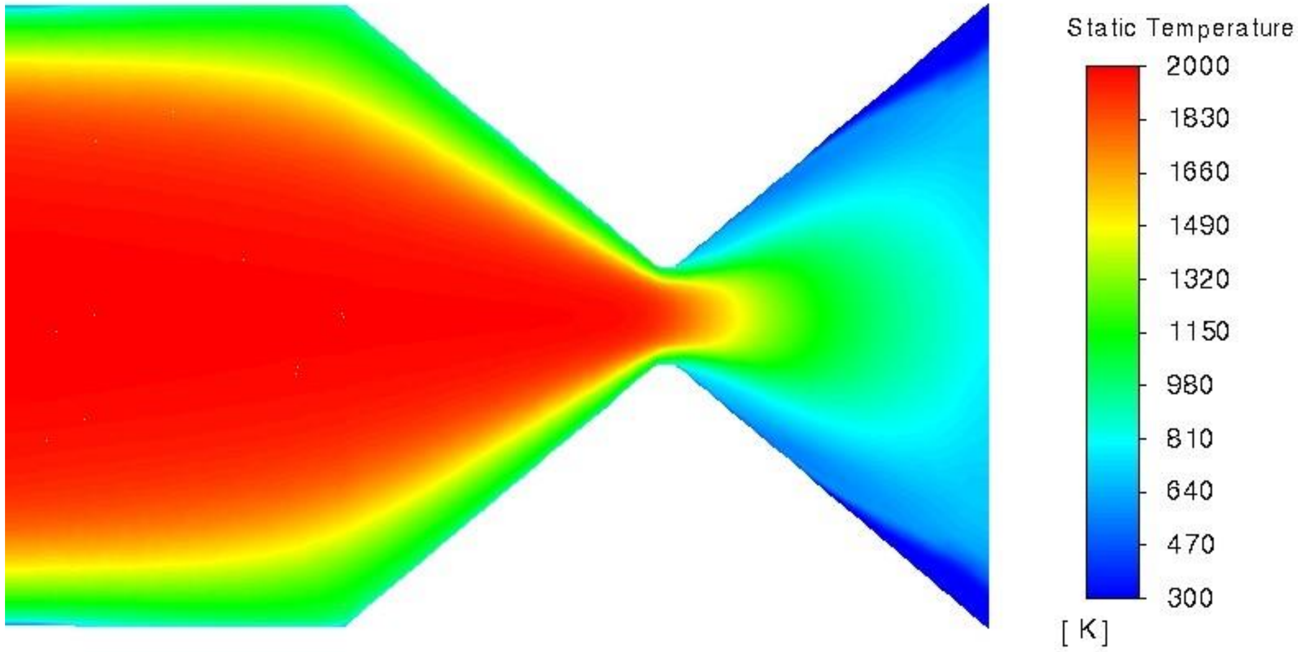
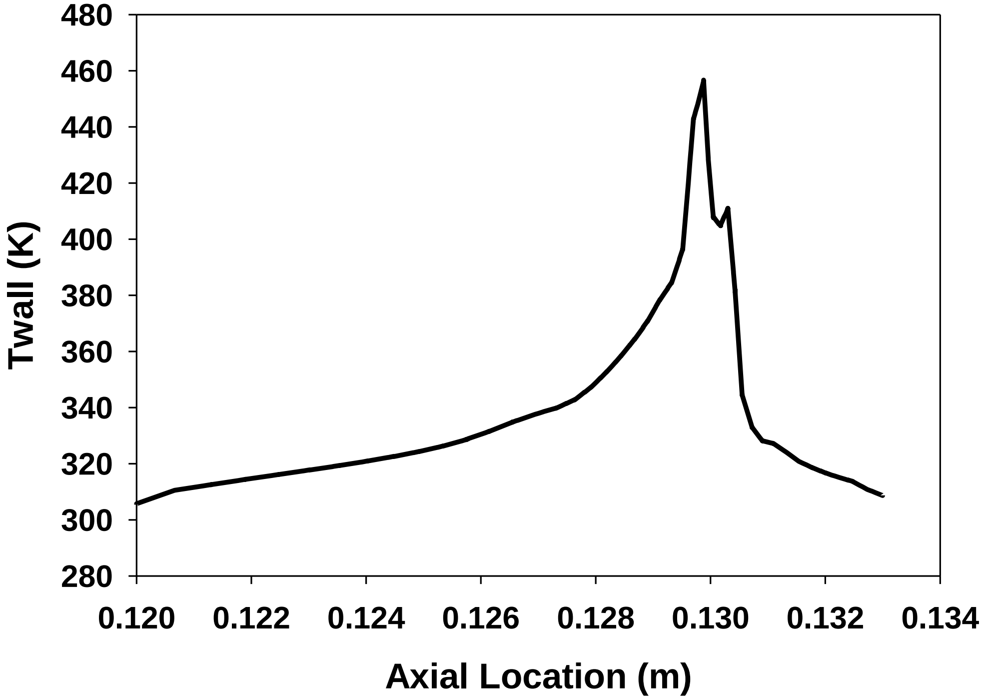
3.175 mm Thick Copper Wall Backside Water Cooled





- **Backside water cooling with copper wall provides effective heat management.**
- **Peak temperature of 460K well below max operating temperature of copper (530K).**

Summary

- Validation of CFD codes and sub-models is needed for high-pressure oxy-combustion conditions.
- Wide range of flame shapes, combustion efficiency and CO production through variation of flowrate, oxidizer preheat temperature and oxidizer swirl.
- Represents a stepping stone to validation at 300 bar pressure (Allam cycle conditions).
- Facility scheduled to be operational by summer 2023.