Oxy-Combustion Fundamentals for Direct Fired Cycles

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Outline

- Effects of pressure and diluents on flames.
- Identification of target conditions.
- Overview of characteristic time and length scales.
- CFD simulations of turbulent time and length scales.
- Chemical kinetic mechanisms.
- Carbon monoxide formation.
- Thermo-acoustic instabilities.

Effect of Pressure on Laminar Flame Speed

- Cantera with GRI 3.0 used to calculate premixed laminar flame speed.
- Flame speed with 31%O2/69%CO2 lower than air mainly due to lower diffusivity.

$$S_L \propto \sqrt{RR \cdot D}$$

$$D \propto {}^{1}/_{P}$$

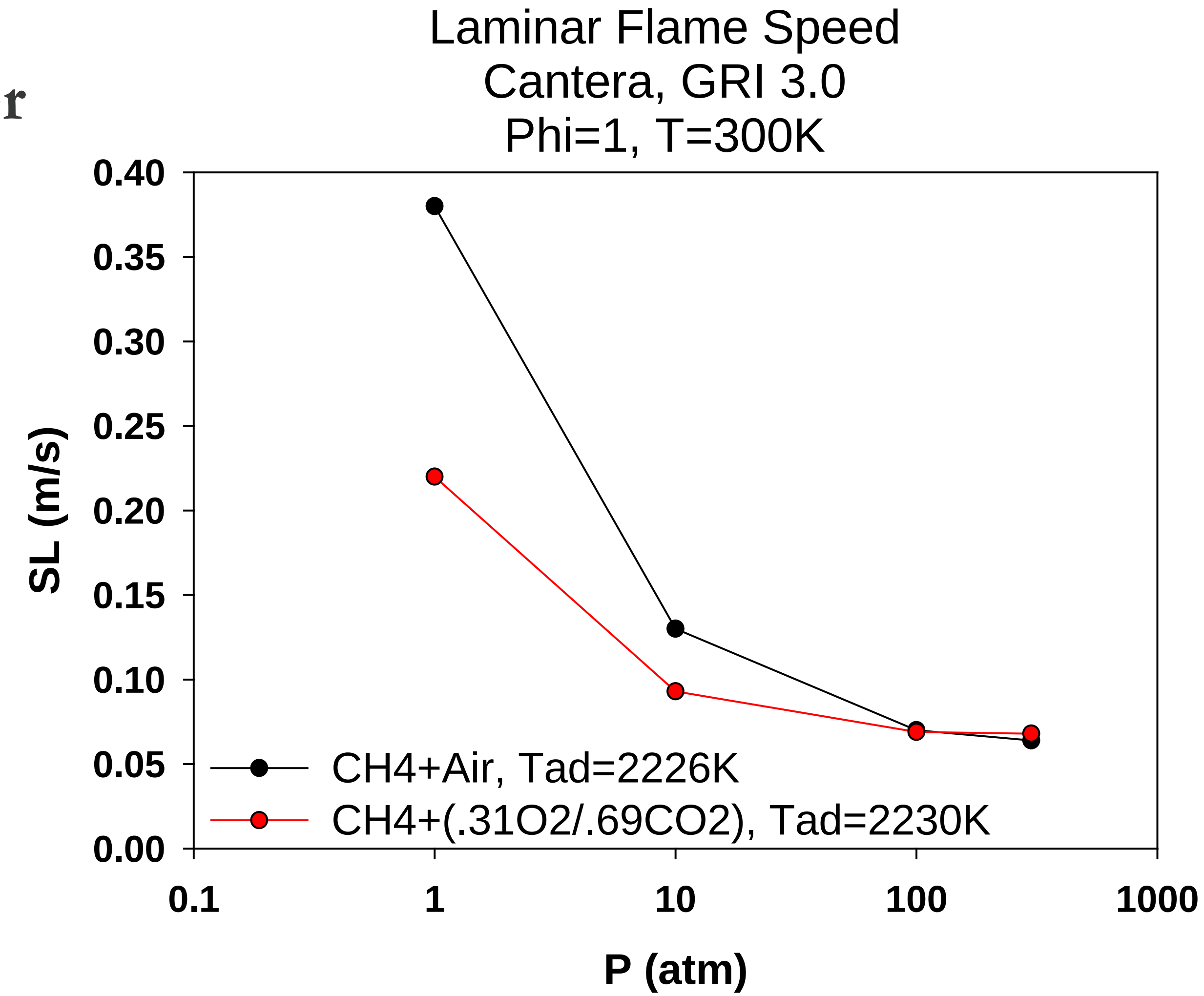
RR= Reaction Rate

D= Molecular Diffusivity

Laminar Flame Thickness

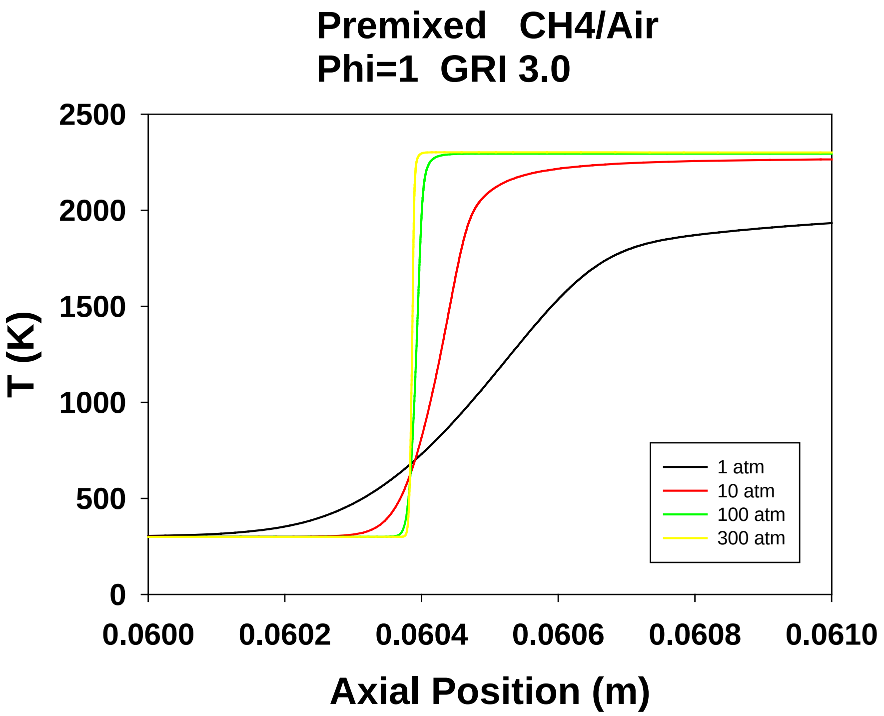
$$\delta_L = \frac{\alpha}{S_L}$$

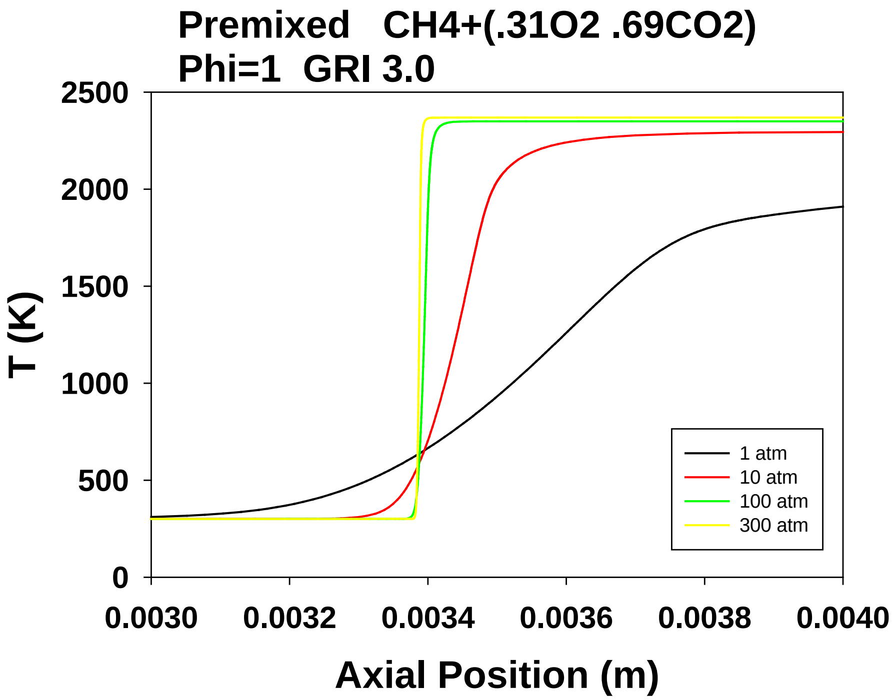
$\alpha = k/\rho C_P$



Cantera Premixed Laminar Flame Profiles

- Temperature profiles through flame region.
- CO2 dilution scaled to provide same equilibrium flame temperature as air flames.

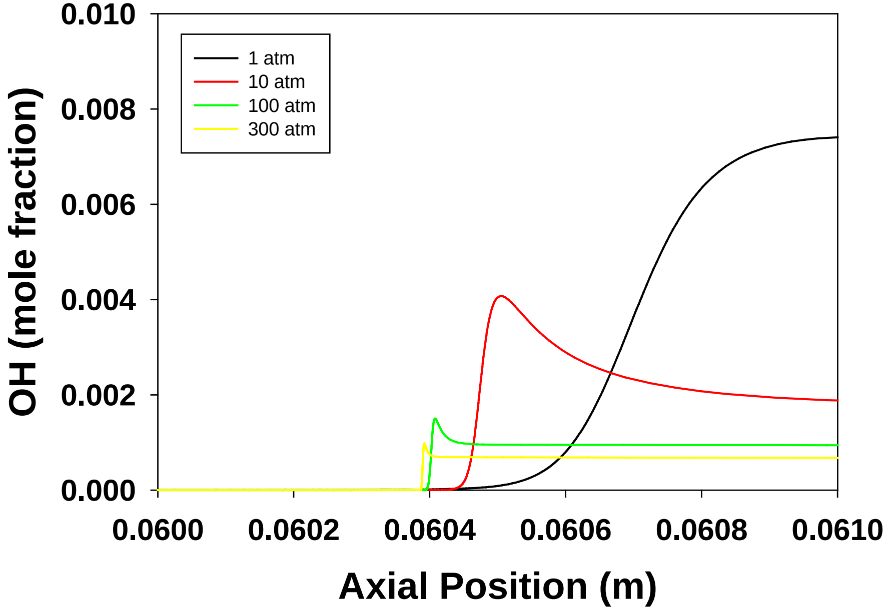

Premixed CH4/Air
Phi=1 GRI 3.0


Premixed CH4+(.31O2 .69CO2)
Phi=1 GRI 3.0

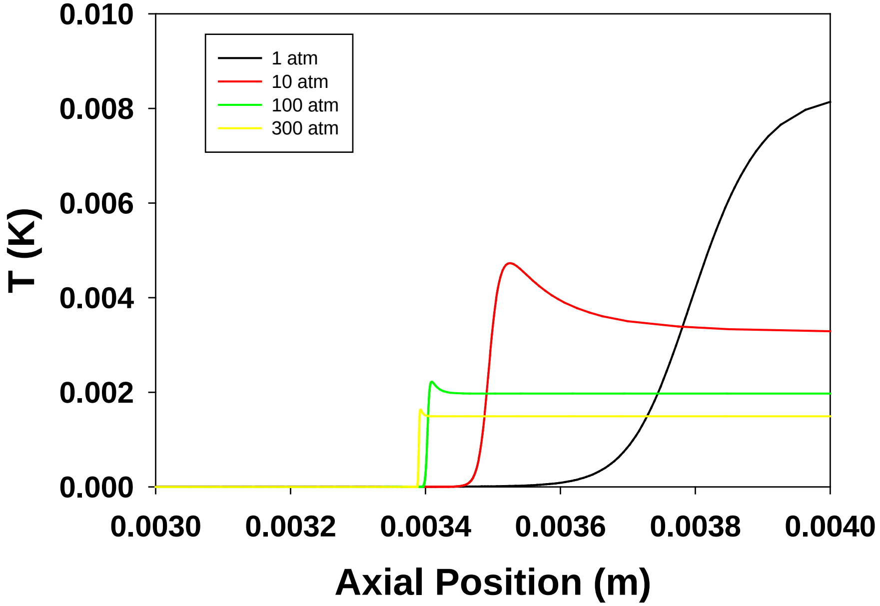
- Flames get much thinner at high pressure.

Cantera Premixed Laminar Flame Profiles

- OH profiles through flame region.
- CO2 dilution scaled to provide same equilibrium flame temperature as air flames.



Premixed CH4/Air
Phi=1 GRI 3.0

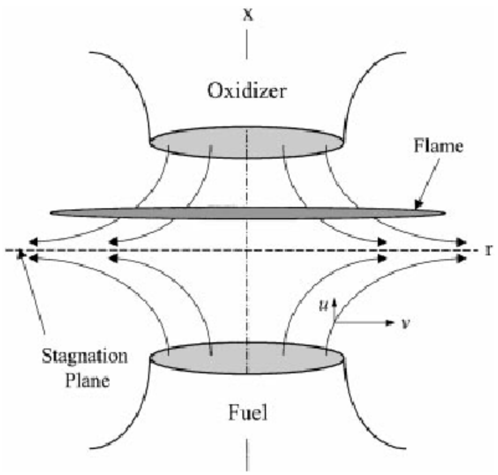


Premixed CH4+(.31O2 .69CO2)
Phi=1 GRI 3.0

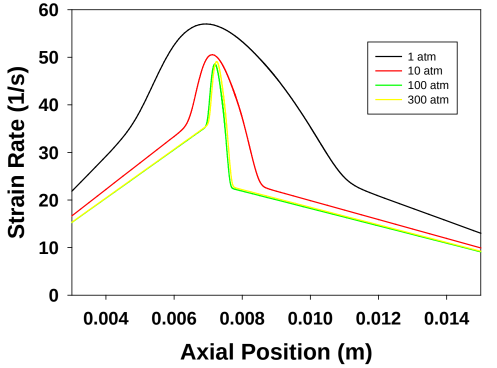
- Radical concentrations reduced at high pressure due to 3-body recombination reactions.

Cantera Non-Premixed Laminar Flame Profiles

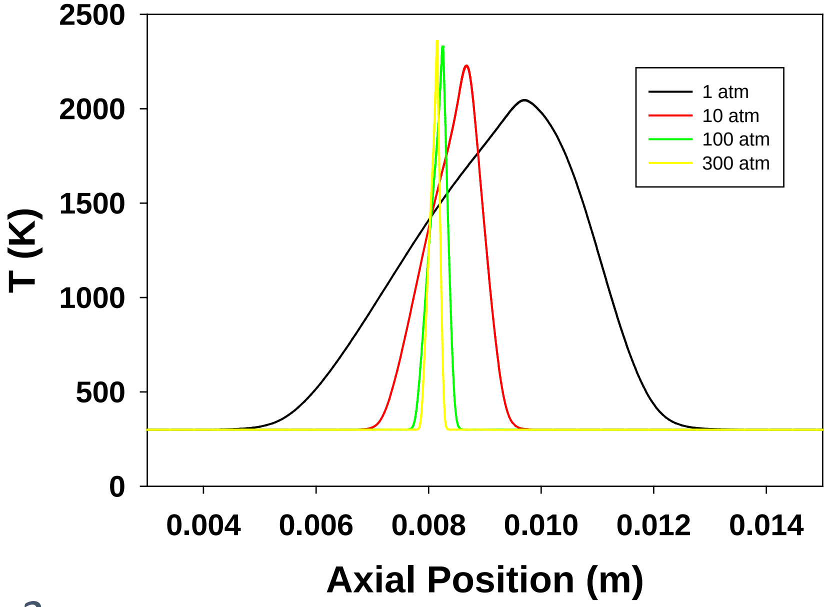
- Temperature profiles through flame region.
- CO2 dilution scaled to provide same equilibrium flame temperature as air flames.



Opposed Diffusion CH4+(.31O2 .69CO2)
Phi=1 GRI 3.0



Opposed Diffusion CH4/Air
Phi=1 GRI 3.0



Opposed Diffusion CH4+(.31O2 .69CO2)
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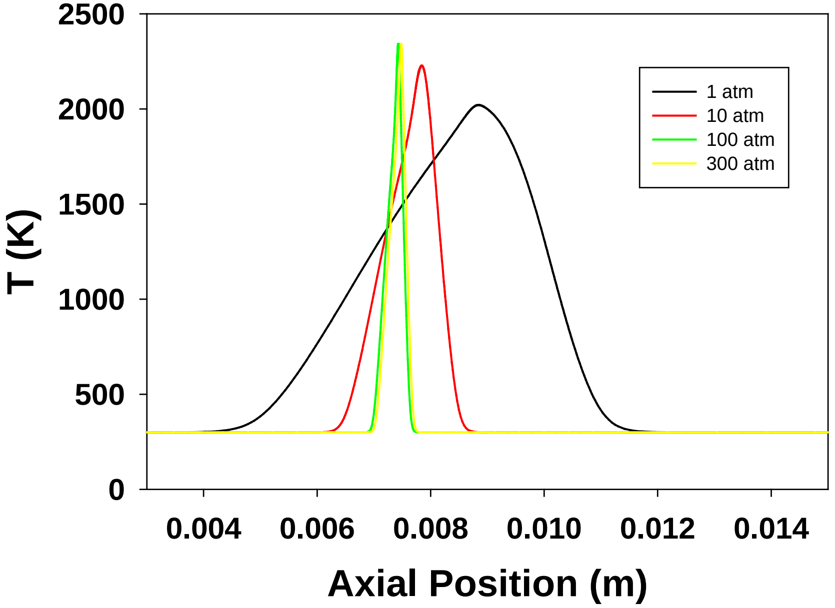
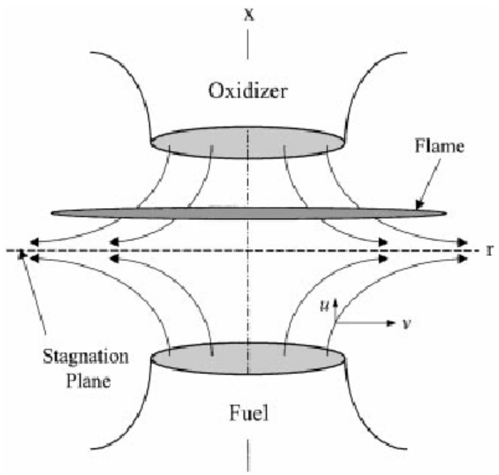


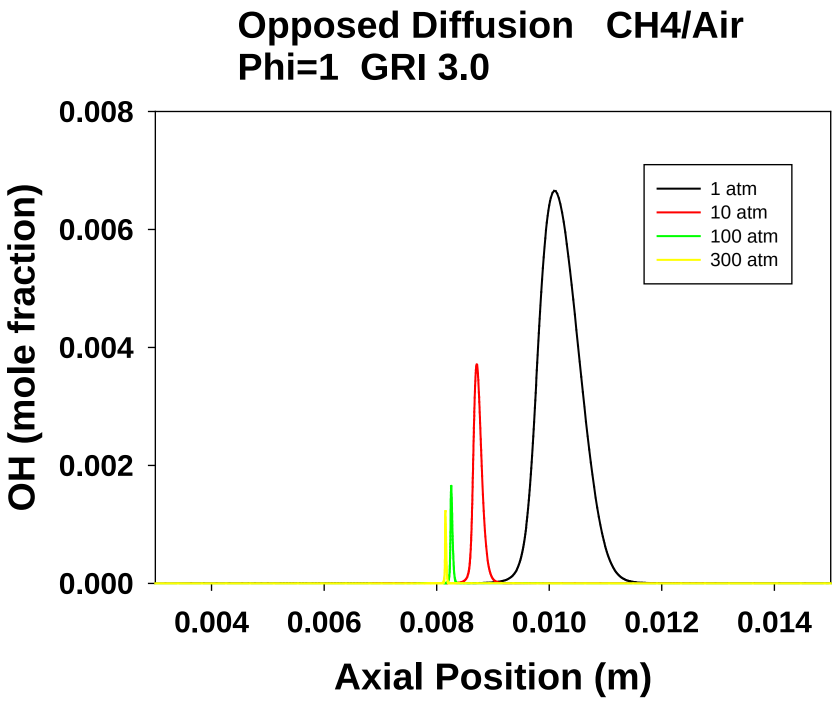
Sep= 2cm

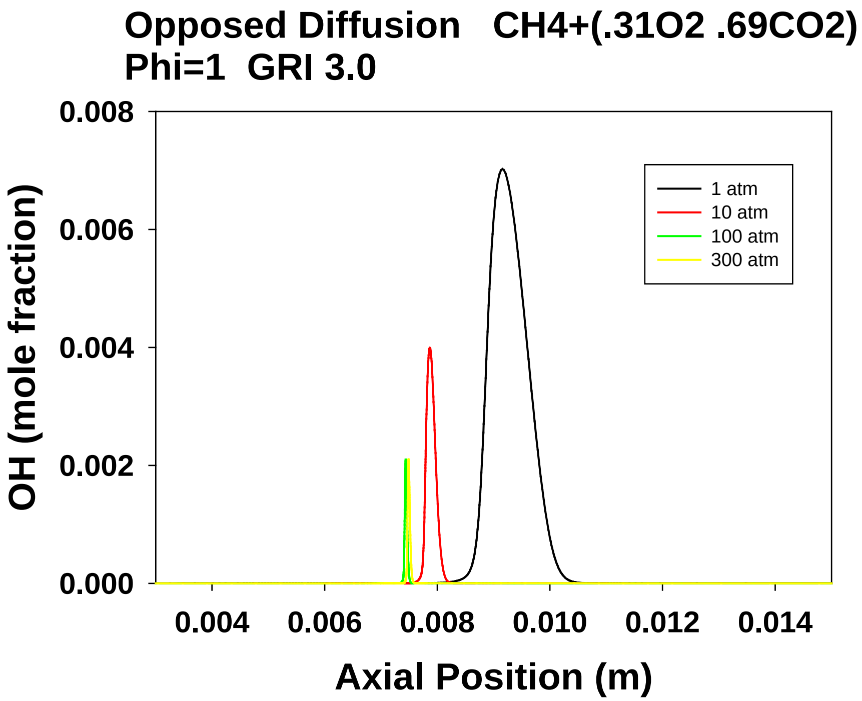
$V_F=V_O=27$ cm/s

Cantera Non-Premixed Laminar Flame Profiles

- OH profiles through flame region.
- CO2 dilution scaled to provide same equilibrium flame temperature as air flames.

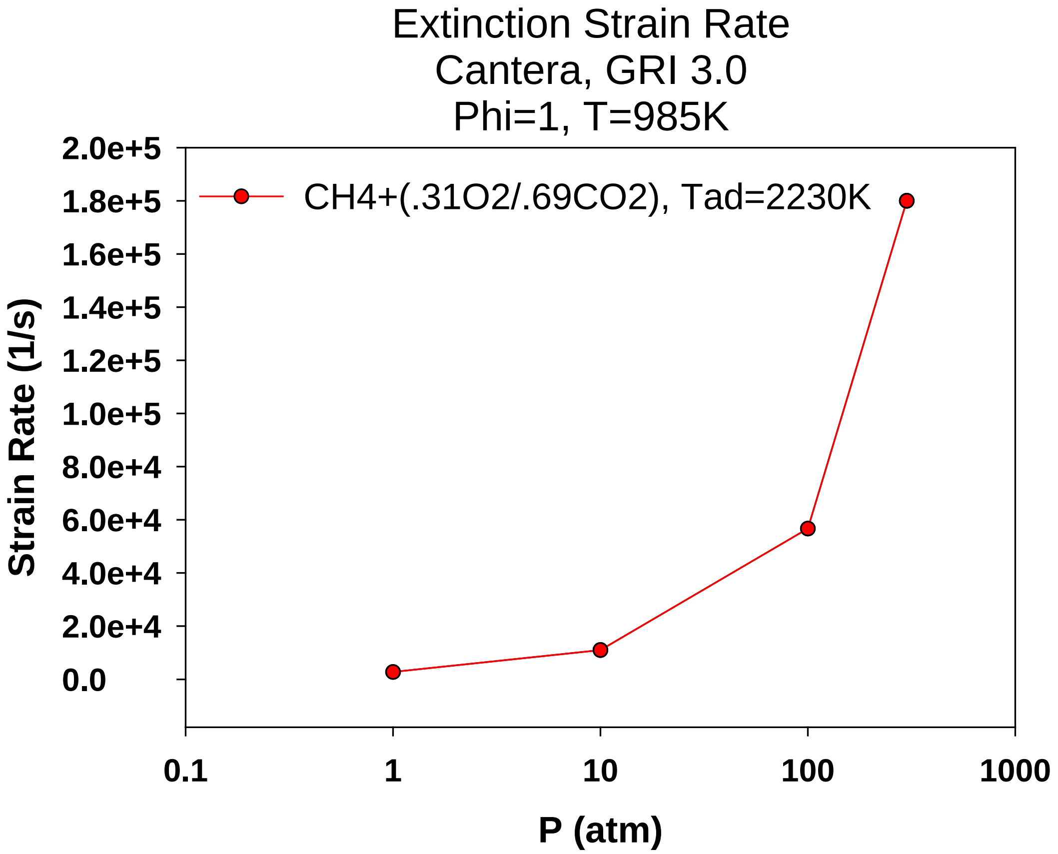


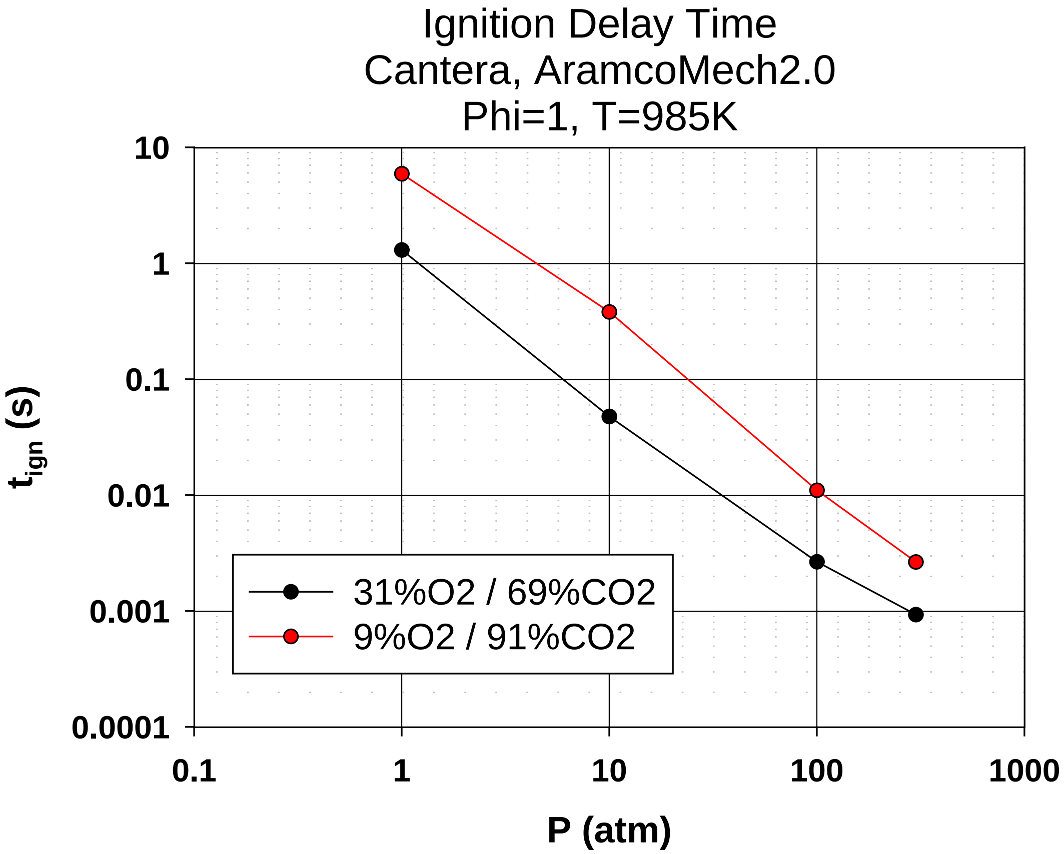




Extinction Strain Rate & Ignition Delay Time

- AramcoMech 2.0 used for ignition delay time.





Allam Cycle

- Goal is to estimate some characteristic combustion scales for high pressure oxy-fuel flames for direct-fired sCO2 cycles.
- Target is the Allam cycle conditions (O_2 15% to 30% molar concentration)*.

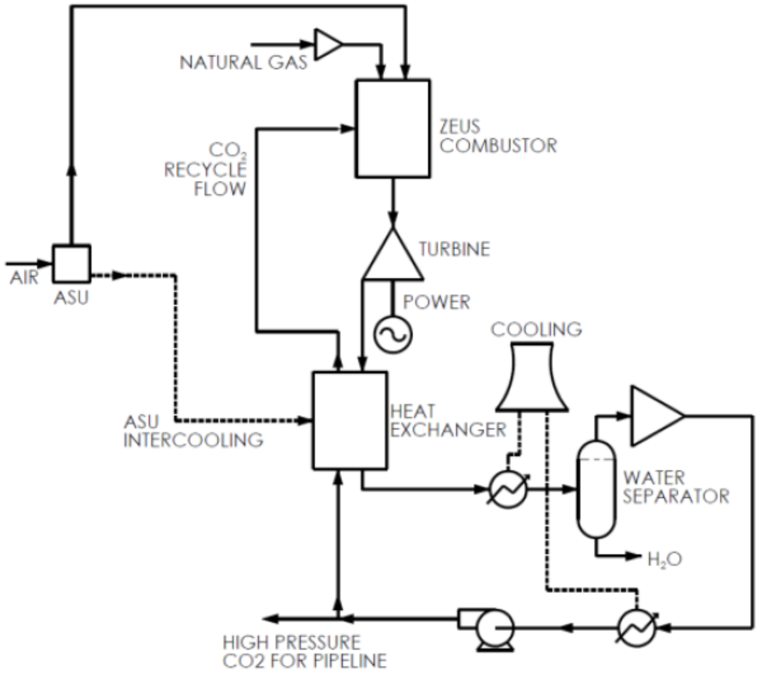


Figure 1. BASIC ALLAM CYCLE NATURAL GAS FLOW DIAGRAM.

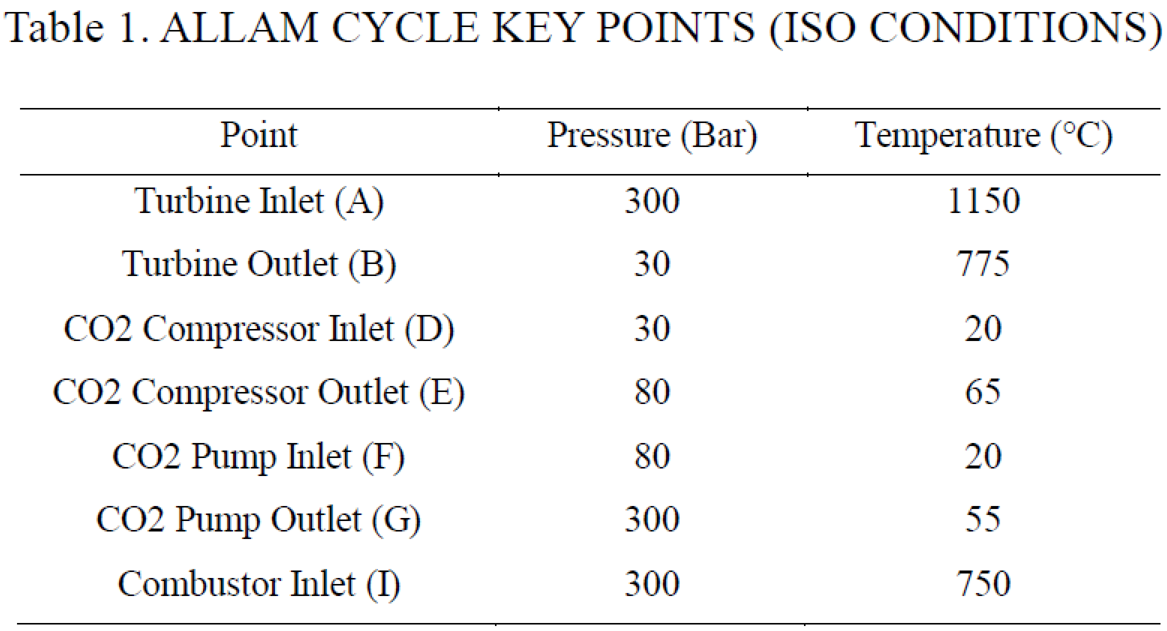


Table 1. ALLAM CYCLE KEY POINTS (ISO CONDITIONS)

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

R.J. Allam et. al., ASME GT2014-26952, 2014

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

Borghi Combustion Diagram

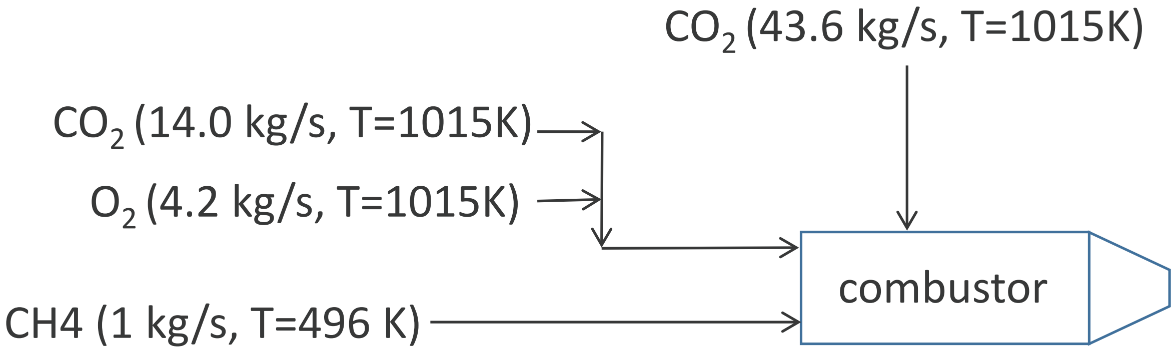
- Borghi Diagram indicates regime of combustion (wrinkled flames, corrugated flames, stirred reactor, etc.

$$need: \frac{u'}{S_L} \; and \; \frac{l_T}{\delta_L}$$

P=300 bar

50 MW Thermal Input

Phi=1.0



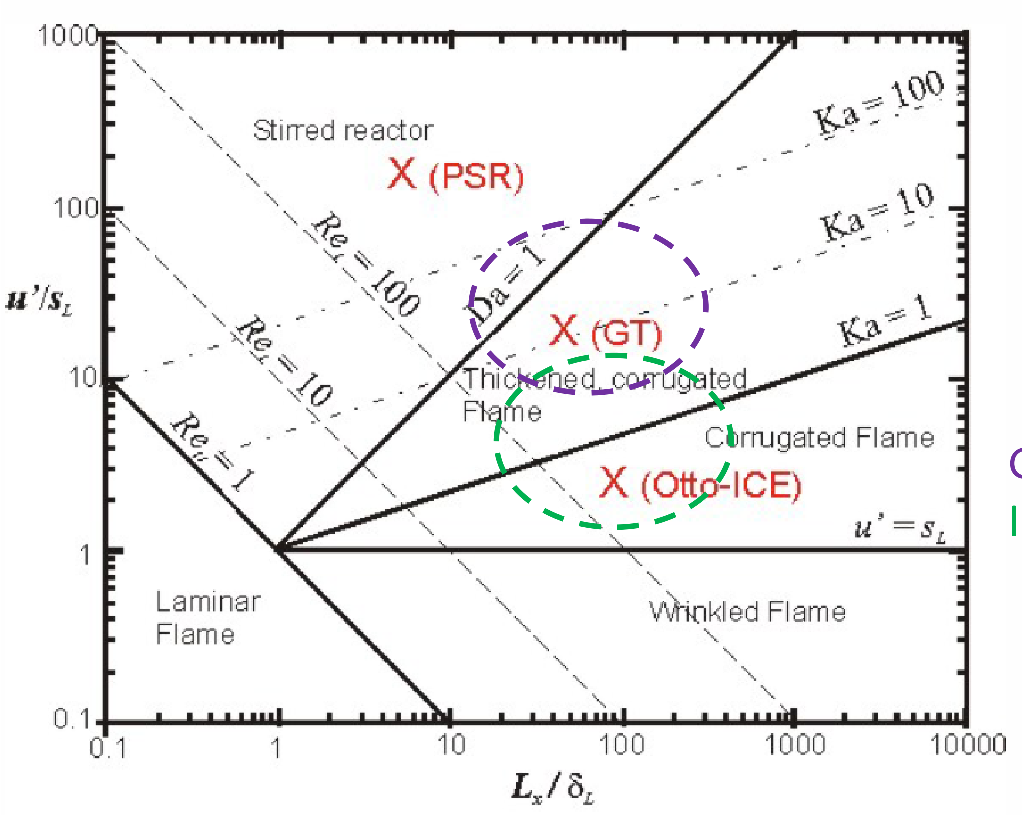
CO_2 (43.6 kg/s, T=1015K)

CO_2 (14.0 kg/s, T=1015K)

O_2 (4.2 kg/s, T=1015K)

CH4 (1 kg/s, T=496 K)

combustor



Gas Turbines

IC Engines

C. Sorusbay, "Turbulent Premixed Combustion in Engines", Istanbul Technical University

Characteristic Scales and Dimensionless Numbers

- **Included here for completeness…**

$Ka = \frac{\tau_{chem}}{\tau_K} = \frac{\delta_L^2}{l_K^2}$ Karlovitz Number (chemical time / Kolmogorov time)

K>1 means the smallest eddies can enter and thicken the flame front

$\mathrm{D}a = \frac{\tau_{turb}}{\tau_{chem}} = .247\left(\frac{k}{\varepsilon}\right)\left(\frac{S_L^2}{\alpha}\right)$ Damkohler Number (turbulent time / chemical time)

Da>>1 means the chemistry is fast compared to turbulent mixing

$\delta_L = \frac{\alpha}{S_L}$ Laminar flame thickness (thermal diffusivity / laminar flame speed)

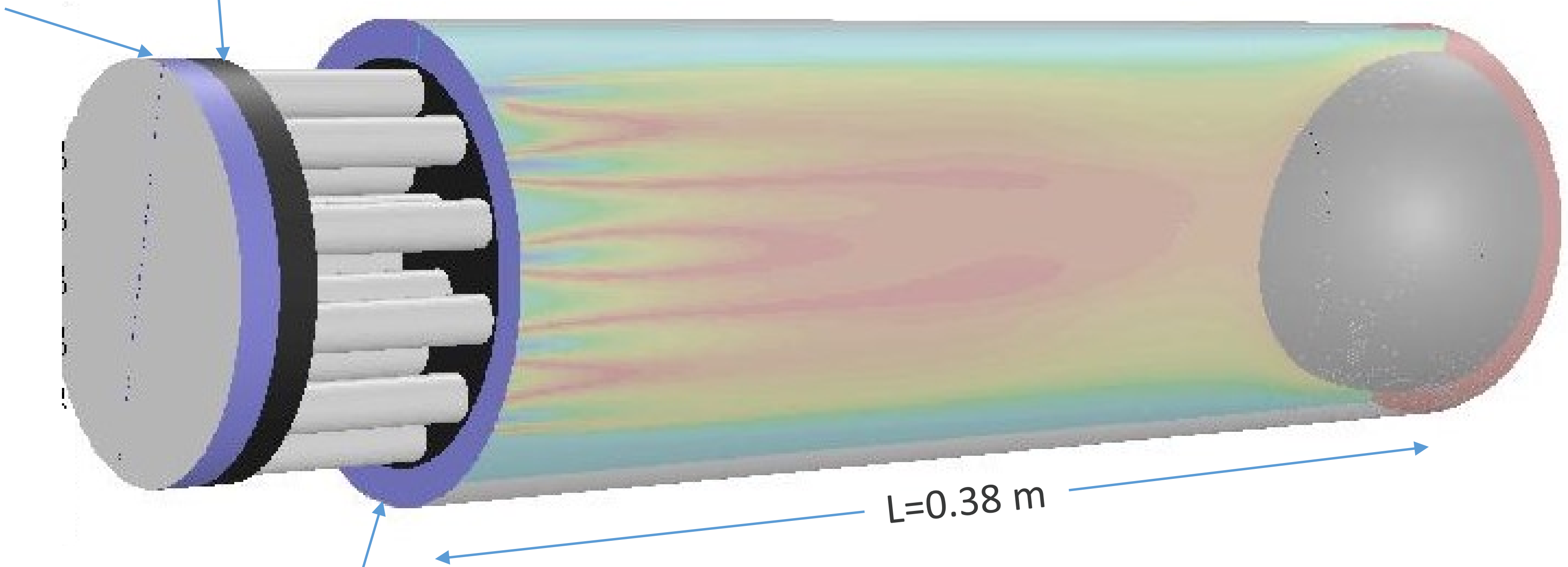
$l_K = \left(\frac{v^3}{\varepsilon}\right)^{1/4}$ Kolmogorov length scale (kinematic viscosity / turbulent dissipation rate)

$l_T = 0.2\frac{k^{1/2}}{\varepsilon}$ Integral length scale (turbulent kinetic energy / turbulent dissipation rate)

$u' = \sqrt{\frac{2k}{3}}$ Turbulent fluctuating velocity

50 MW Conceptual Combustor

SSME Preburner type combustor – 21 coaxial injectors, 4M Cells



Oxidizer in

CO_2 (12.6 kg/s, T=1015K)

O_2 (4.2 kg/s, T=1015K)

Fuel in

CH4 (1 kg/s, T=496 K)

D=0.125 m

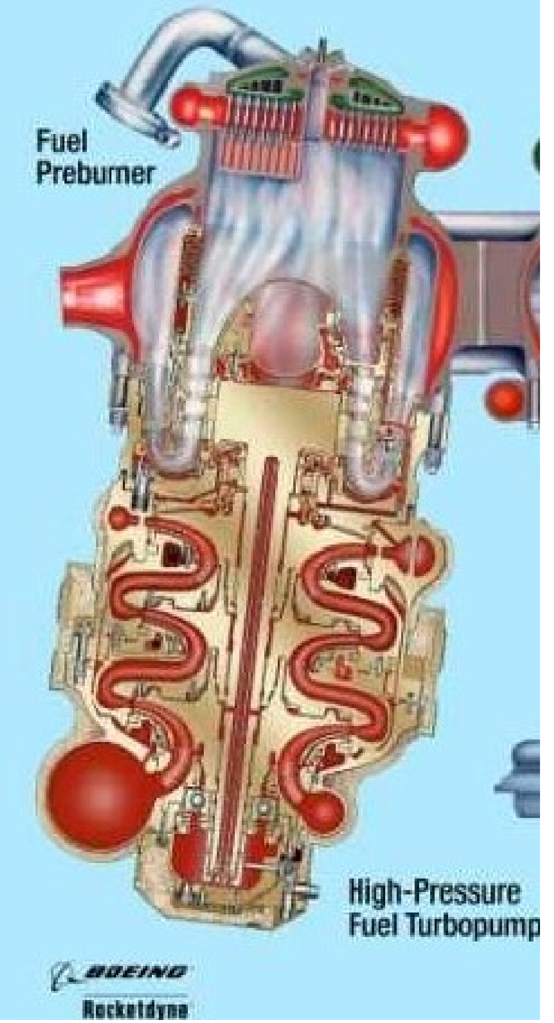
L=0.38 m

Purge in

CO_2 (43.6 kg/s, T=1015K)

P=300 bar

50 MW Thermal Input



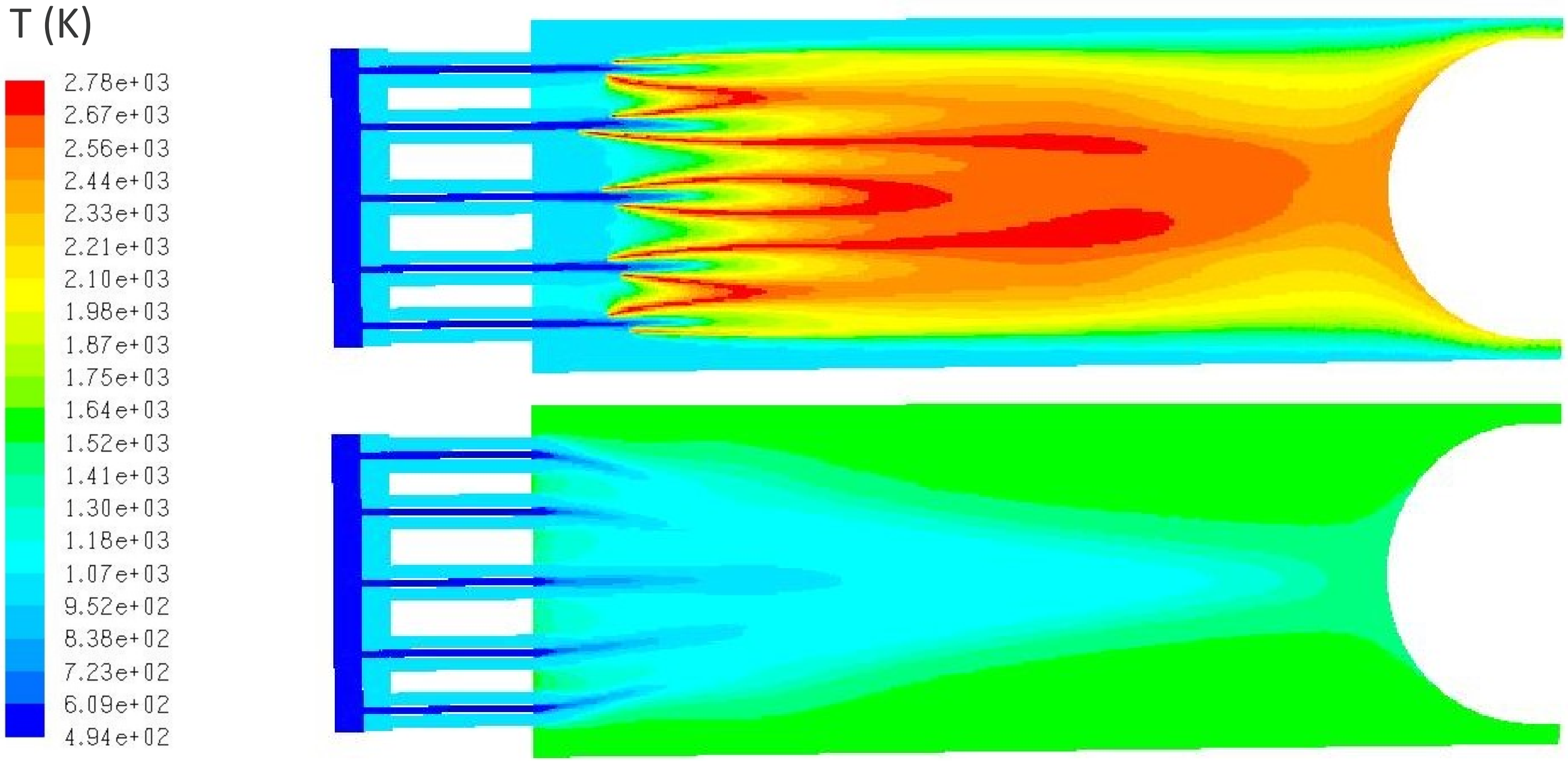
Turbulent Time and Length Scales

Two Limiting Cases:

1) 25% of CO2 by mass mixed in with O2 (X_{O2}=0.30, ϕ=1.0)

2) Fully mixed (100% of CO2 mixed in with O2) (X_{O2}=0.09, ϕ=1.0)

Steady RANS k-e
DRM19 reduced CH4 mechanism
No Combustion model



25% of CO2 with O2 (X_{O2}=0.30)
75% of CO2 through purge
l_T=1.9 mm
U'=7.5 m/s

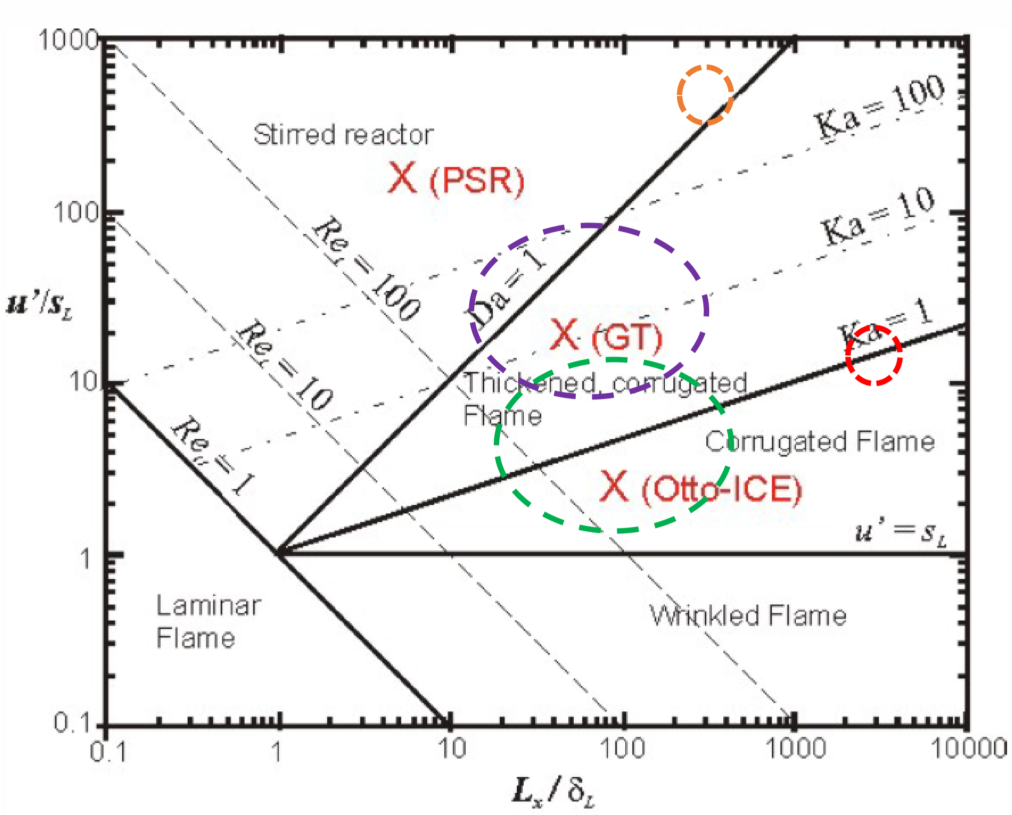
100% of CO2 with O2 (X_{O2}=0.09)
l_T=2.0 mm
U'=23.8 m/s

Borghi Diagram for Oxy-Combustion

- Two cases shown for 300 bar oxy-combustion define a range of conditions spanning the thickened, corrugated flame regime and stirred reactor.

- Significantly outside the range of gas turbine and IC engine operation.

- Requires assessment of appropriate turbulent combustion models.



Gas Turbines

IC Engines

300 bar sCO2 (.31O2+.69CO2)
S_L = 0.58 m/s (T_F=2690K)
δ_L = 0.67 μm
Ka=0.7
Tign=9.2e-4 s

300 bar sCO2 (.09O2+.91CO2)
S_L = 0.05 m/s (T_F=1610K)
δ_L = 6.60 μm
Ka=361
Tign=2.5e-3 s

Potential Range of Operating Conditions

- 30% O2 case looks like a conventional turbulent flame.
- 9% O2 case looks like autoignition.

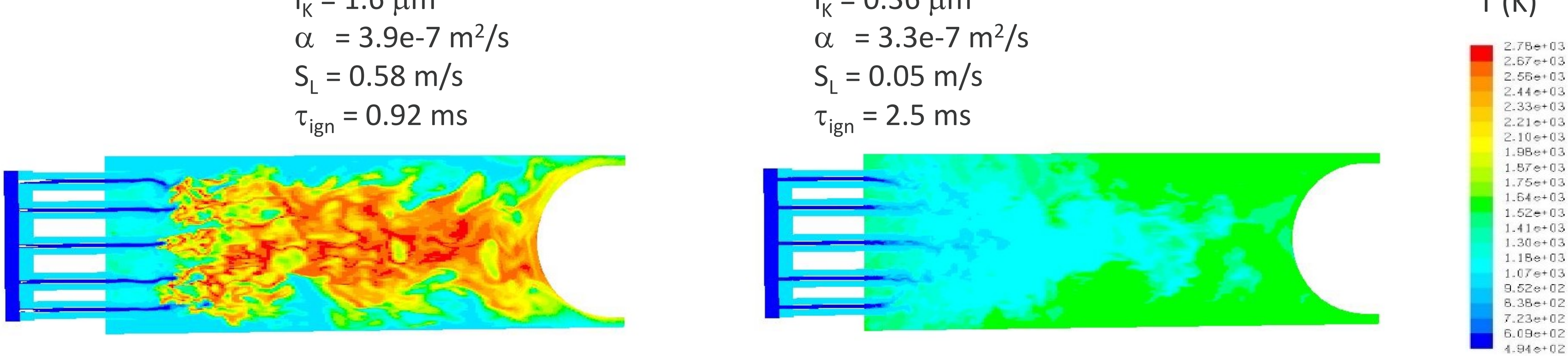
<u>30%O2/70%CO2</u>

$U = 30$ m/s
$\tau_R = 12.7$ ms
$\tau_T = 2.6\text{e-}4$ s
$l_T = 1.9$ mm
$\tau_K = 3.4\text{e-}6$ s
$l_K = 1.6\ \mu\text{m}$
$\alpha = 3.9\text{e-}7\ \text{m}^2/\text{s}$
$S_L = 0.58$ m/s
$\tau_{ign} = 0.92$ ms

<u>9%O2/91%CO2</u>

$U = 50$ m/s
$\tau_R = 7.6$ ms
$\tau_T = 9.3\text{e-}5$ s
$l_T = 2.0$ mm
$\tau_K = 4.1\text{e-}7$ s
$l_K = 0.36\ \mu\text{m}$
$\alpha = 3.3\text{e-}7\ \text{m}^2/\text{s}$
$S_L = 0.05$ m/s
$\tau_{ign} = 2.5$ ms

Large Eddy Simulations



Chemical Kinetic Mechanisms

- No detailed mechanisms validated at sCO2 conditions. Best available is likely Aramco Mech (U. Galway). Validated with flame-speed up to 60 bar and ignition delay to 260 bar. Likely better than GRI 3.0.
- Huge mechanism, 103 species, 480 reactions after reduction to C2 and smaller.
- Need for compact skeletal mechanisms amenable to CFD modeling (10-30 species maximum).

Need flame speed, species profiles and induction time data for direct-fired conditions!

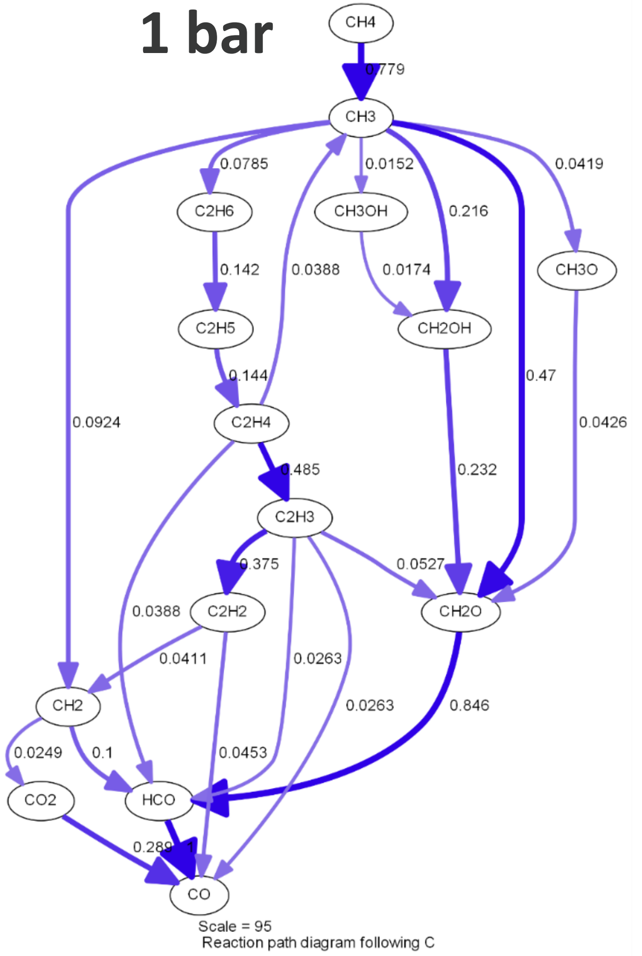
Mechanism Reduction

Reaction Path Analysis, 0-D Reactor

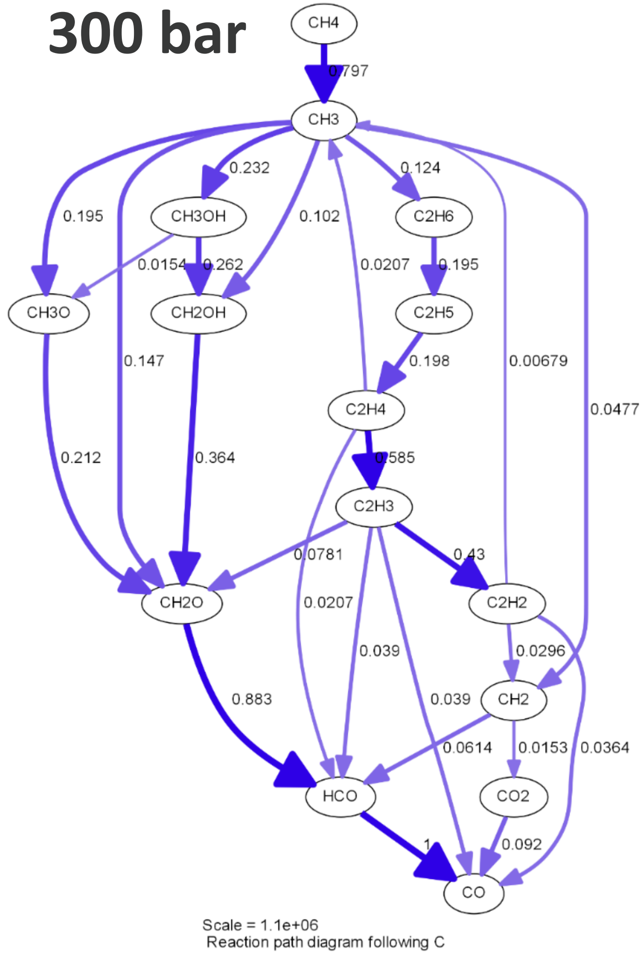
T=985K, CH4=.12989, O2=.27351, CO2=.5966

- Methane oxidation kinetics very different at 300 bar.
- More reaction paths play an important role, therefor larger skeletal mechanisms needed to adequately represent kinetics.

1 bar



300 bar

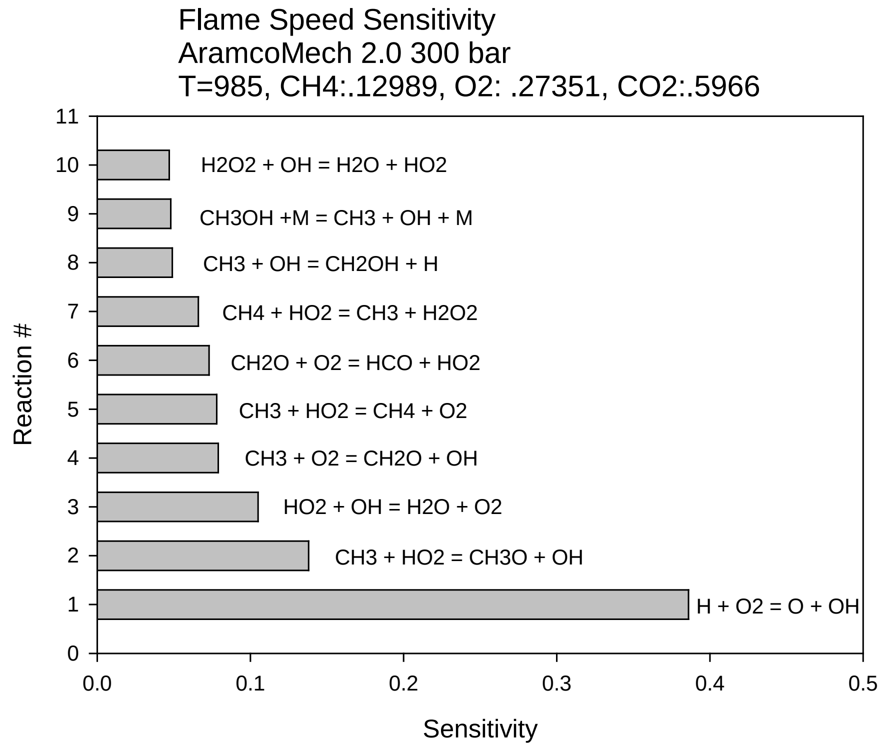


Mechanism Reduction

- Combination of reaction path analysis, flame-speed sensitivity and ignition delay time sensitivity.
- Optimized for Allam cycle combustor conditions
  - 300 bar
  - $T_{preheat} \sim 1000K$
  - Oxidizer: 25% O_2 + 75% CO_2

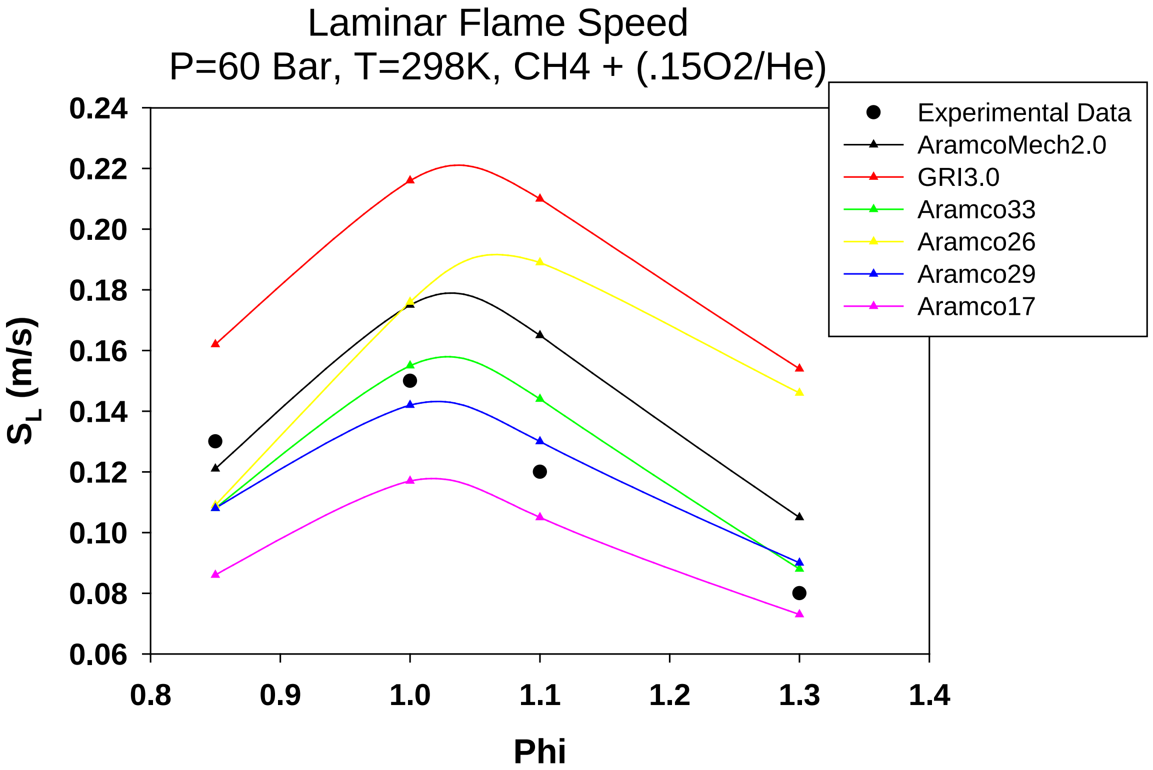
- Several skeletal mechanisms developed with 33, 29, 26 and 17 species.

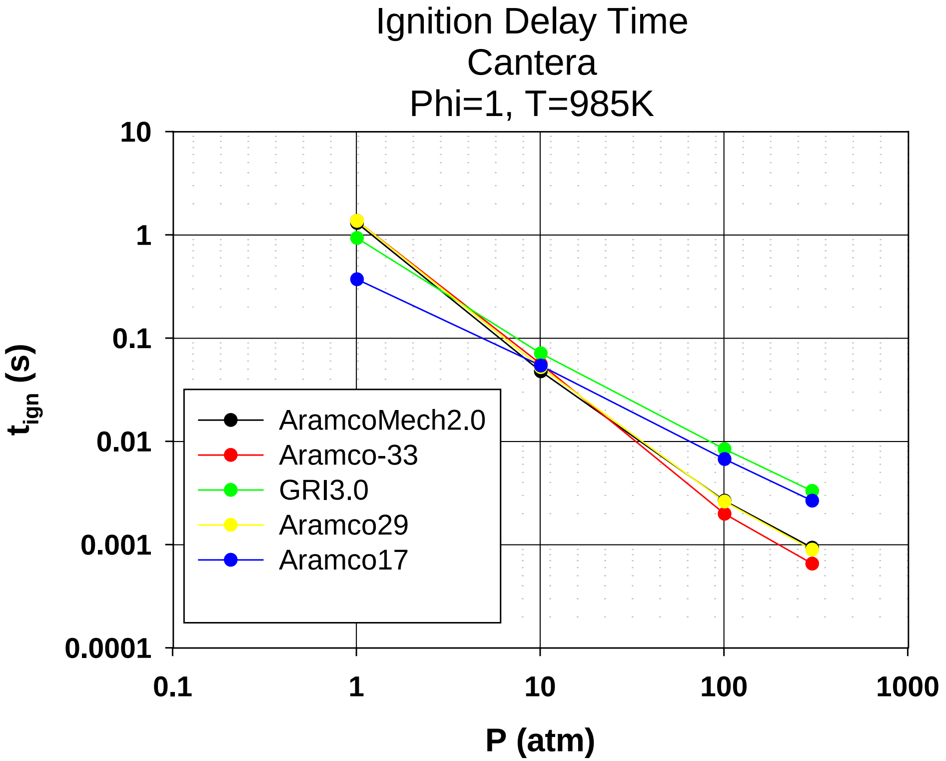
Flame speed sensitivity at 300 bar



Mechanism Reduction

- **Performance comparison of various skeletal mechanisms.**
  - Flame speed and ignition delay improve with the inclusion of more species and reactions.
    - 33 and 29 species able to predict flame-speed and ignition delay very well.
    - 17 species able to predict flame-speed to within ~40% error.

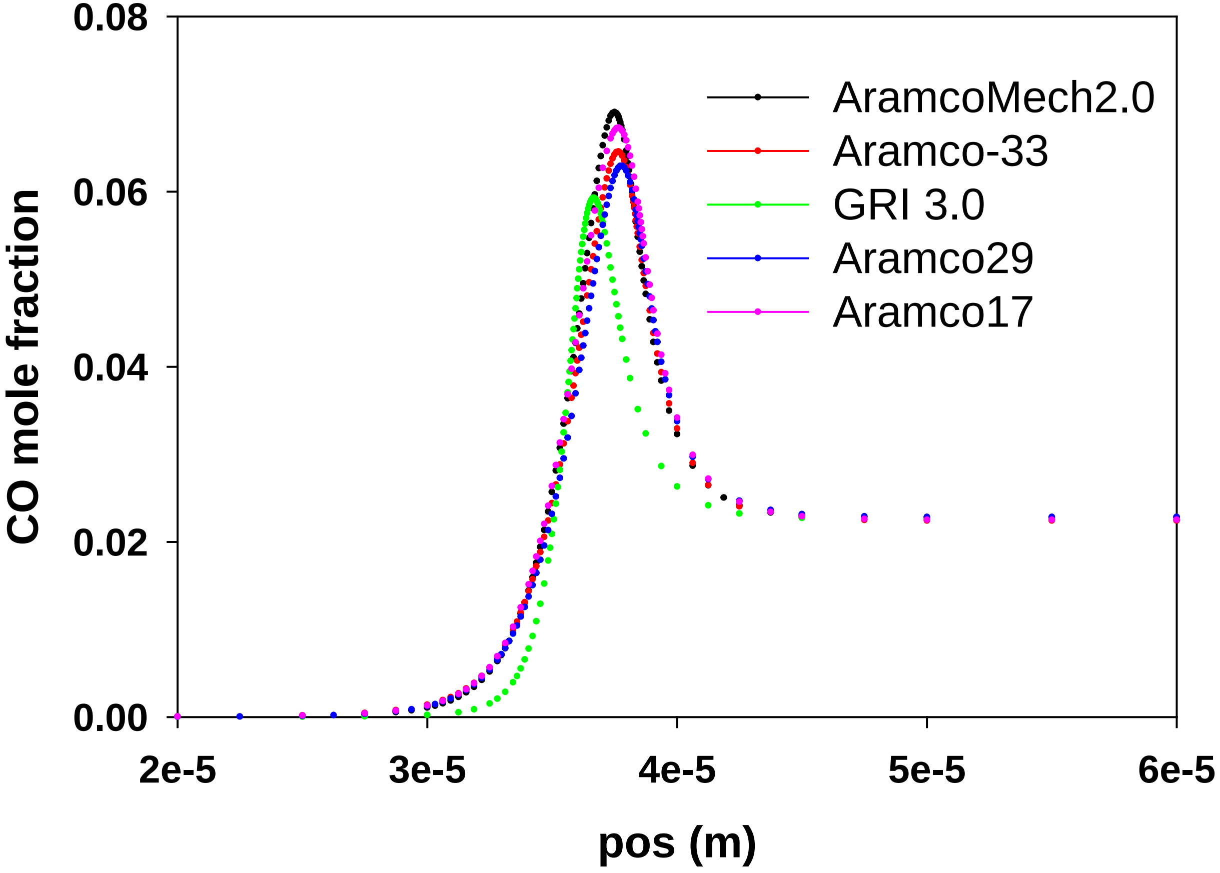




Mechanism Reduction

- **Performance comparison of various skeletal mechanisms.**
  - All do very well for CO production profiles.
- **CO prediction important for accurate cycle efficiency calculations.**

Laminar Flame Profiles
P=300 bar, T=995K
CH4=.12989, O2=.27351, CO2=.5966



Estimation of CO Production

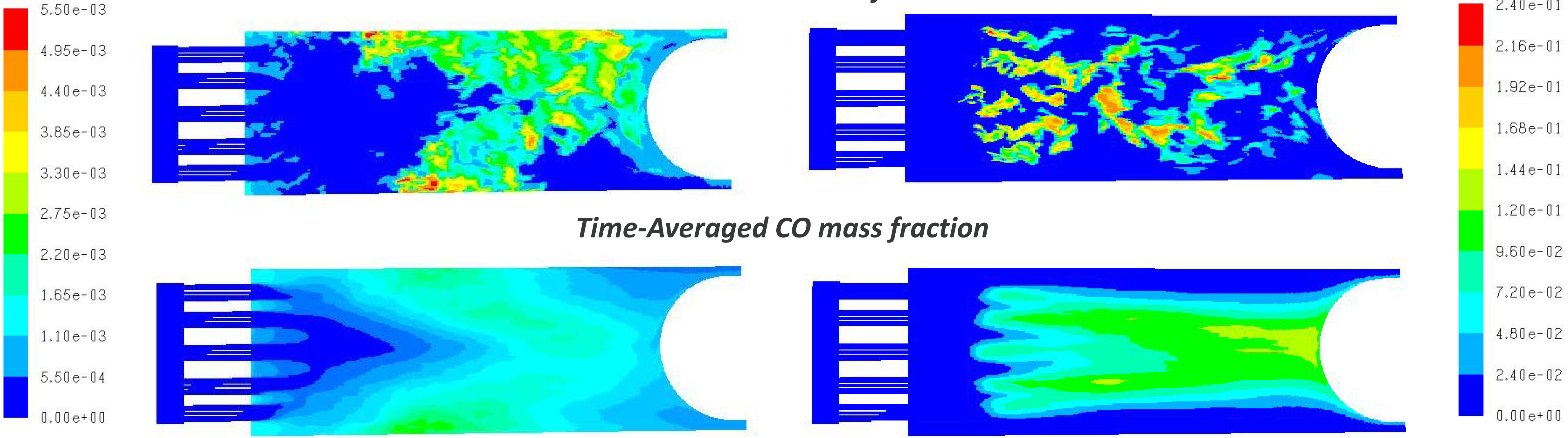
Large Eddy Simulation, Dynamic Smagorinksy
17-species skeletal mechanism
FDF Combustion Model, Modified Curl, C_M=2

Equilibrium Calcs
Flame (30% O2) : X_{CO}=.024
Comb Exit: X_{CO} = 1.2e-5

9%O2/91%CO2, ϕ=1.0 ***30%O2/70%CO2, ϕ=1.0***

Instantaneous CO mass fraction

Time-Averaged CO mass fraction

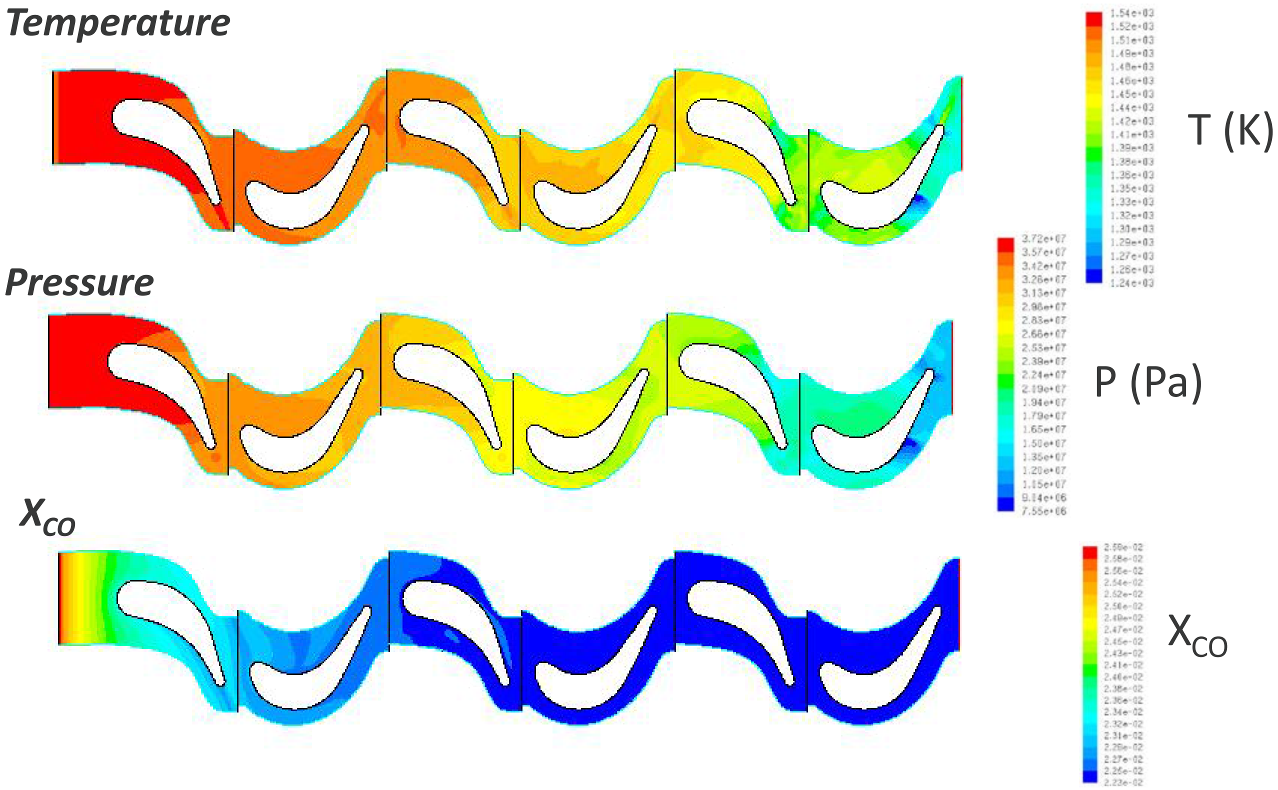


X_{CO}=.00098

X_{CO}=.026

Fate of CO in Turbine

RANS, SST-kOmega, DRM19, V_{blade}=150 m/s, Pr=2.85



Equilibrium Calcs

Flame: X_{CO}=.024 (30% O2, **ϕ**=1.0)
Comb Exit: X_{CO} = 1.2e-5

Simulation Results

Inlet: X_{CO}=.026
Outlet: X_{CO}=.023

- CO concentration is well above equilibrium at turbine inlet conditions.
- CO oxidation reactions are slow relative to residence time in turbine.
- CO is effectively “frozen” at flame conditions.

Effect of CO on sCO2 Cycle Efficiency

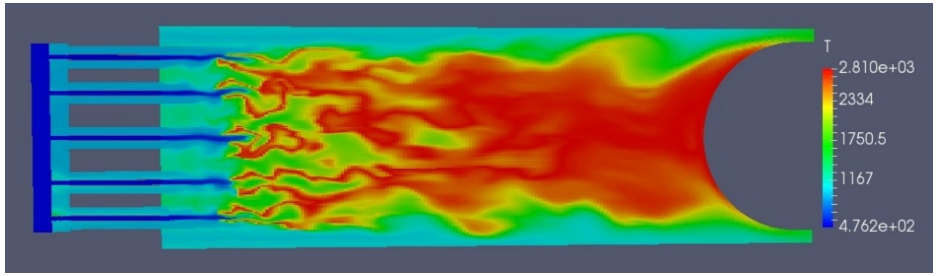
- Preliminary cycle calculations indicate as much as a 1.6 percentage point decrease in cycle thermal efficiency per mole percentage of CO in the combustor exhaust.
- Drop off in cycle and process efficiency is due to an increase in compression power as a result of CO in working fluid.

Source: NETL SEA (Chuck White)

Modeling Thermo-Acoustic Instabilities

- **Aramco17 (17 species, 45 reactions)**
- **50 mW (1 kg/s CH_4 flow).**
- **Oxidizer 25%O_2 + 75%CO_2 by mass.**
- **3M cells, LES model**

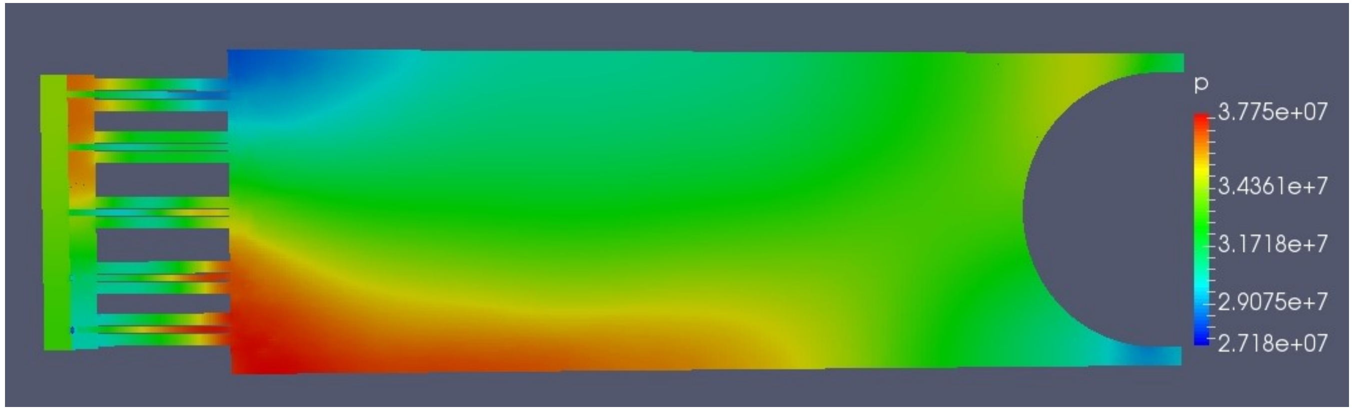
OpenFOAM LES, pressure-based solver



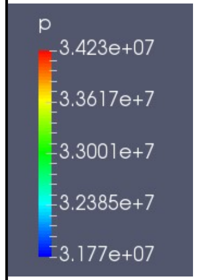
Radial mode thermoacoustic instability @ 3kHz.

Peak-to-Peak pressure oscillation 60% of mean combustor pressure.

Pressure Field (Pa)



Slice at Z=2 cm



Concluding Remarks

- **Oxy-combustion at 300 bar is somewhat uncharted territory.**
  - Conditions more representative of rocket engines.
  - Limited data available.
- **Need for validated detailed chemical kinetic mechanisms as well as reduced mechanisms.**
- **Must take care in selecting appropriate combustion models (fast mixing, flamelet, EDC, PDF, etc…).**
- **CO levels must be kept low ($X_{CO} < .0015$) for maximum cycle efficiency.**
- **Thermo-acoustic stability must be assessed.**
  - Modeling can help.
  - Passive devises (baffles, Helmholtz resonators) may be necessary.