Investigation of Methane and Syngas Autoignition at High Pressure Conditions

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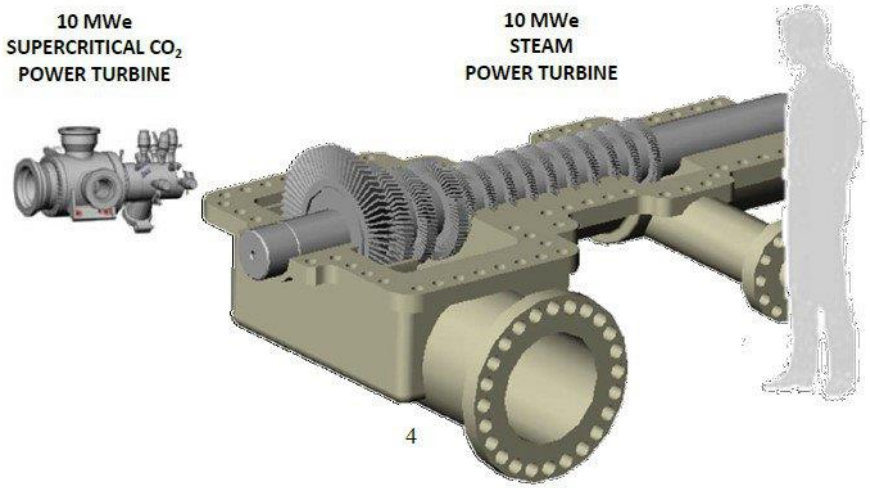
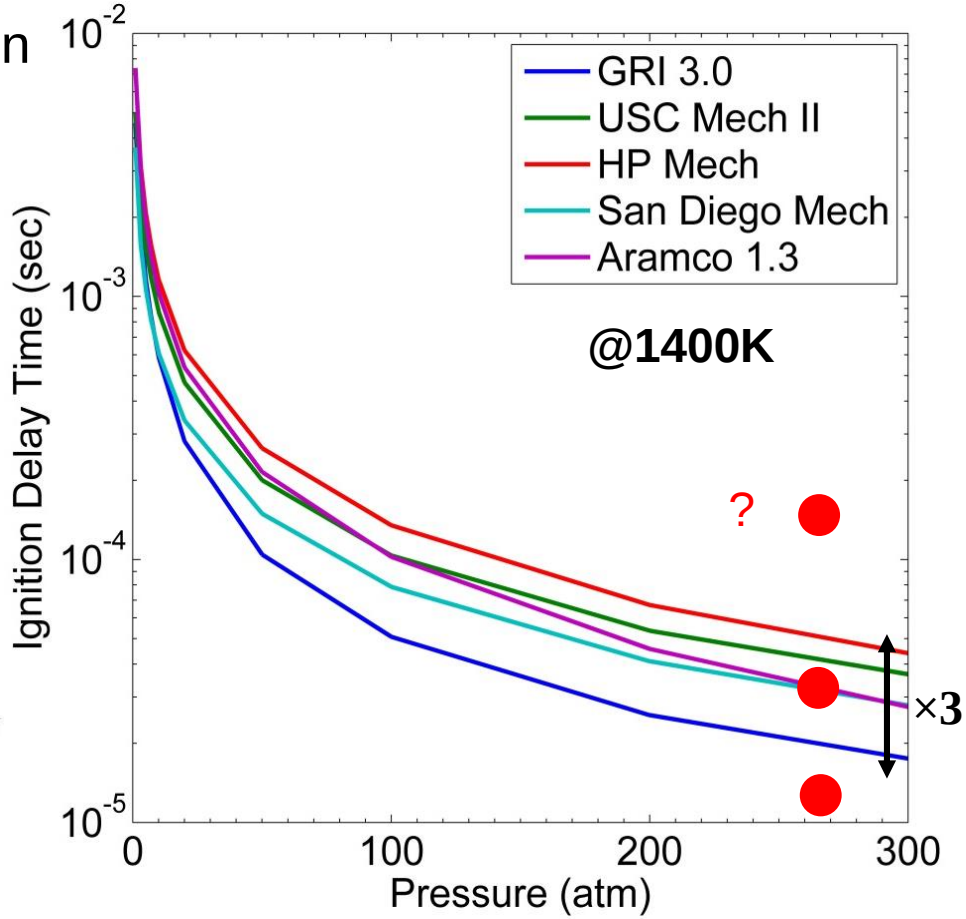
Background

- Technology driven
  - Supercritical CO_2 oxy-combustion
    - high efficiency, ~100% carbon capture
  - Completely new operating condition
    - 100-300 atm
- Bridge the knowledge gap

Compact but more efficient system



Echogen's 10 MWe sCO_2 power turbine compared to a 10 MWe steam turbine.



$CH_4/O_2/CO_2$ (9.5%:19%:71.48%)

GT High Pressure Shock Tube

Key features:

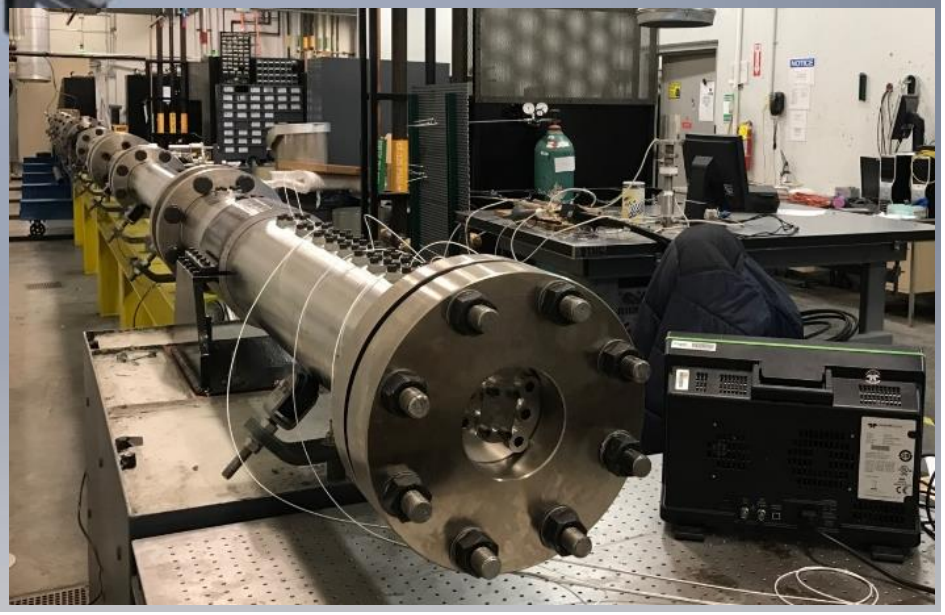
- Large internal bore (6 inch or 15.24 cm)
- 69 ft long (~50 ms test time)
- Certified at 376 atm
- 0.2 μm surface finish (electropolishing)
- Optical access

Diaphragm section (single or double)

Eight optical windows

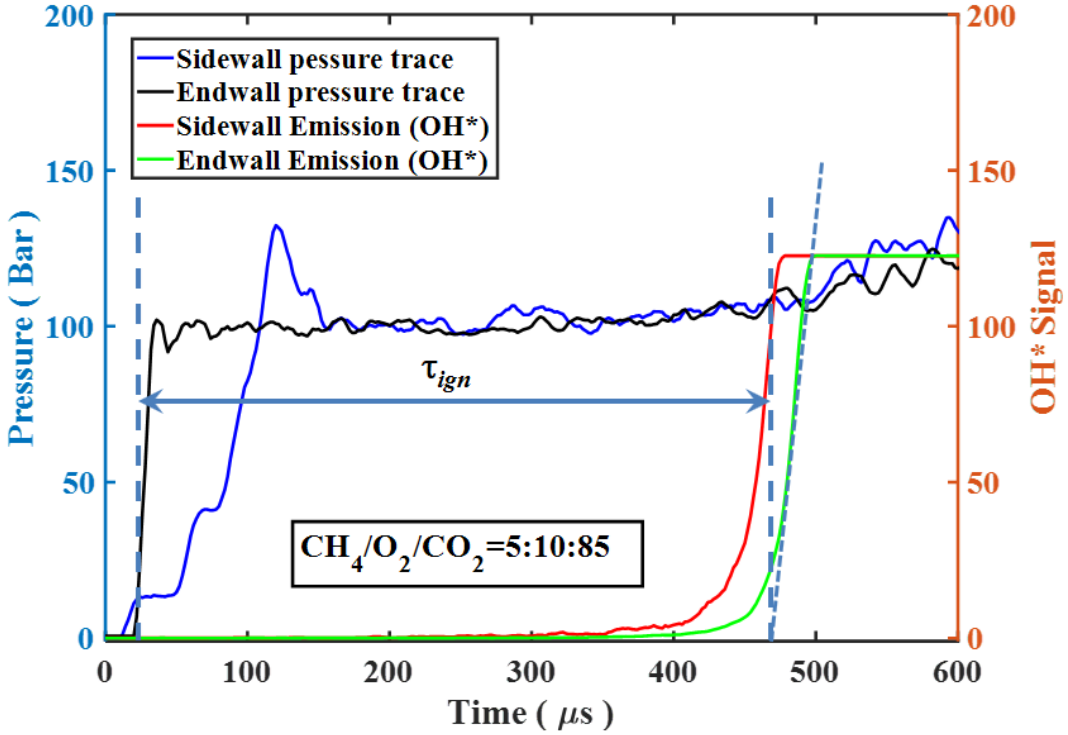
Contoured valve for vacuum

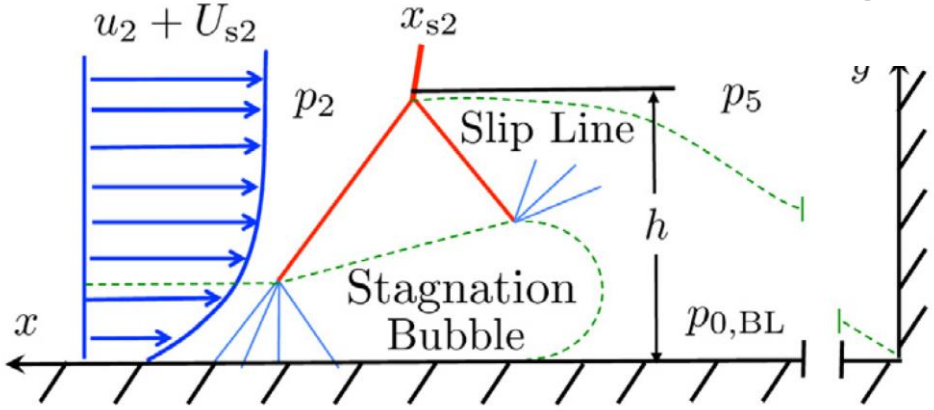
Single piece test section (2.1 m)



Challenges of Experiments at sCO_2 Condition

- Large C_p of CO_2
  - Strong shock needed for CO_2
- BL is much thicker with CO_2
  - Non-ideal effect
- **ID of shock tube must be larg**
  - **150 mm**
  - **High experimental cost**

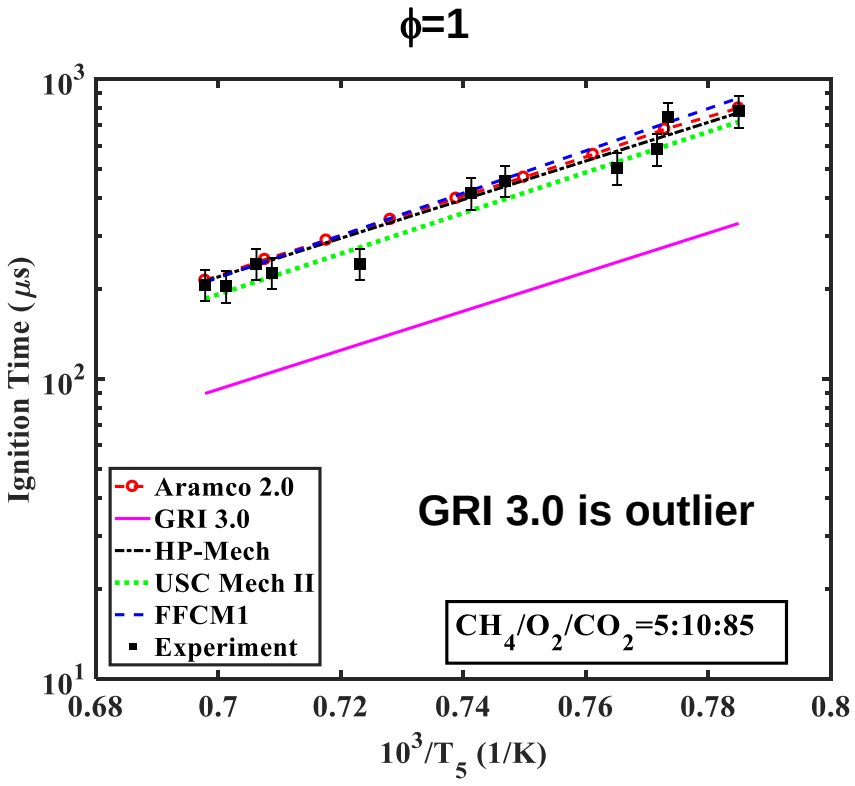


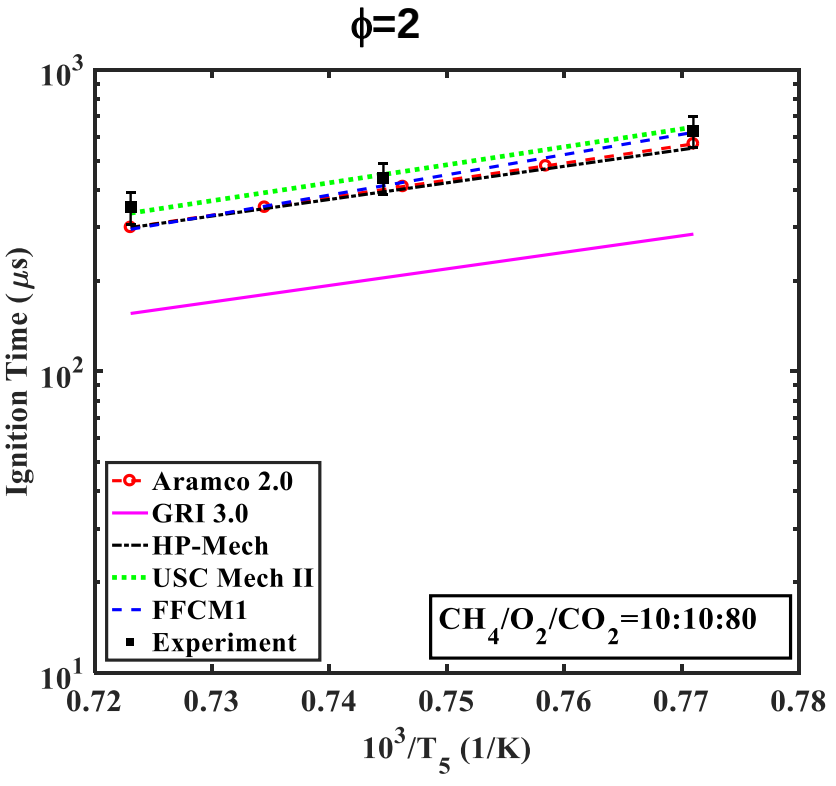


K. Grogan & M. Ihme, PROCI, 2016

Autoignition Delays at sCO_2 condition

- **Pressure: 100±5 bar**, and **temperature range of 1274 to 1433 K**

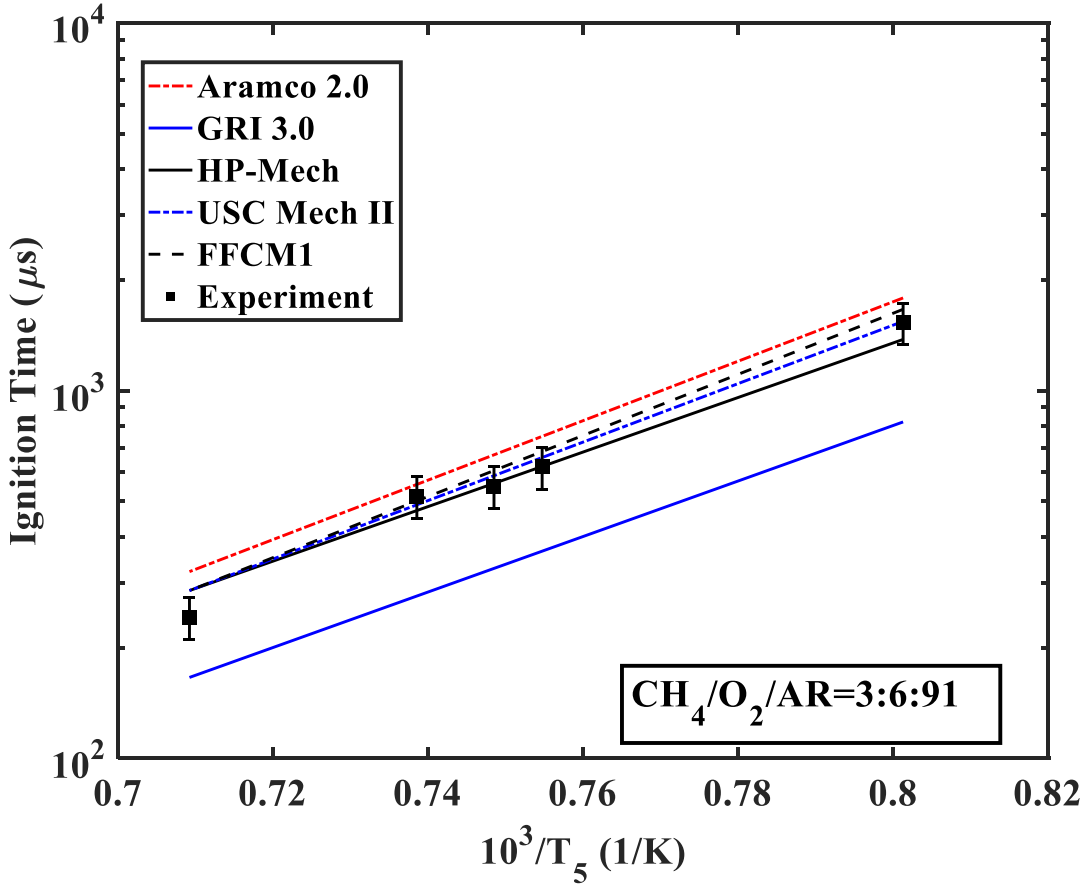




Simulation results from Aramco 2.0, USC Mech II and HP-Mech are close to each other, however GRI 3.0 predicts a significantly shorter autoignition delay, having approximately a **factor of 3 difference**

Autoignition Delays of CH_4 in Ar

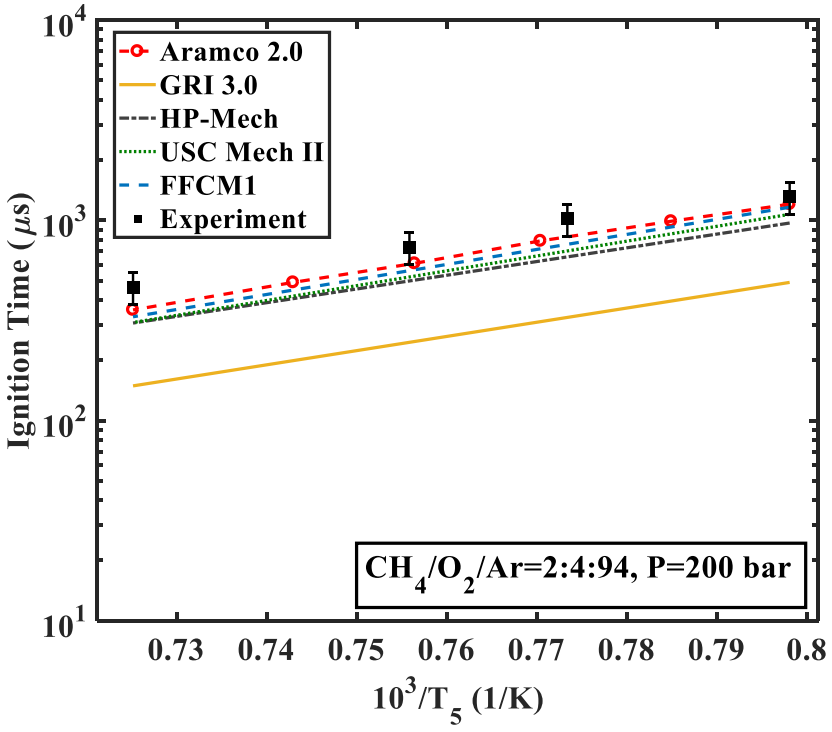
- **Pressure: 95±3 bar**, and **temperature range of 1248 to 1410 K**

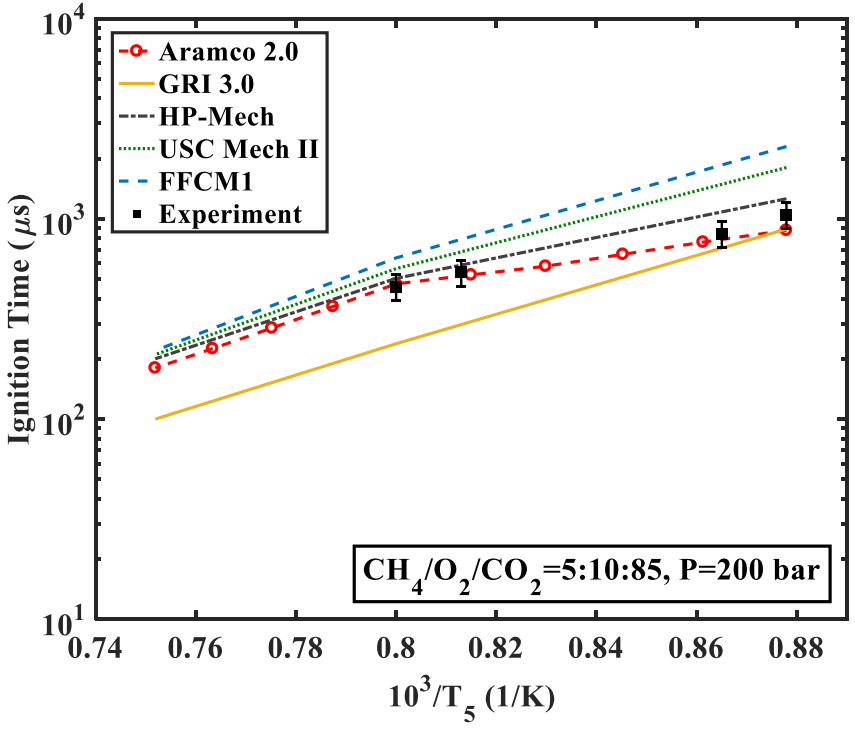


No chemical effect from diluent is observed

Autoignition Delays of CH_4 in CO_2 and Ar

- **Pressure: 200±5 bar**, and **temperature range of 1137 to 1380 K**



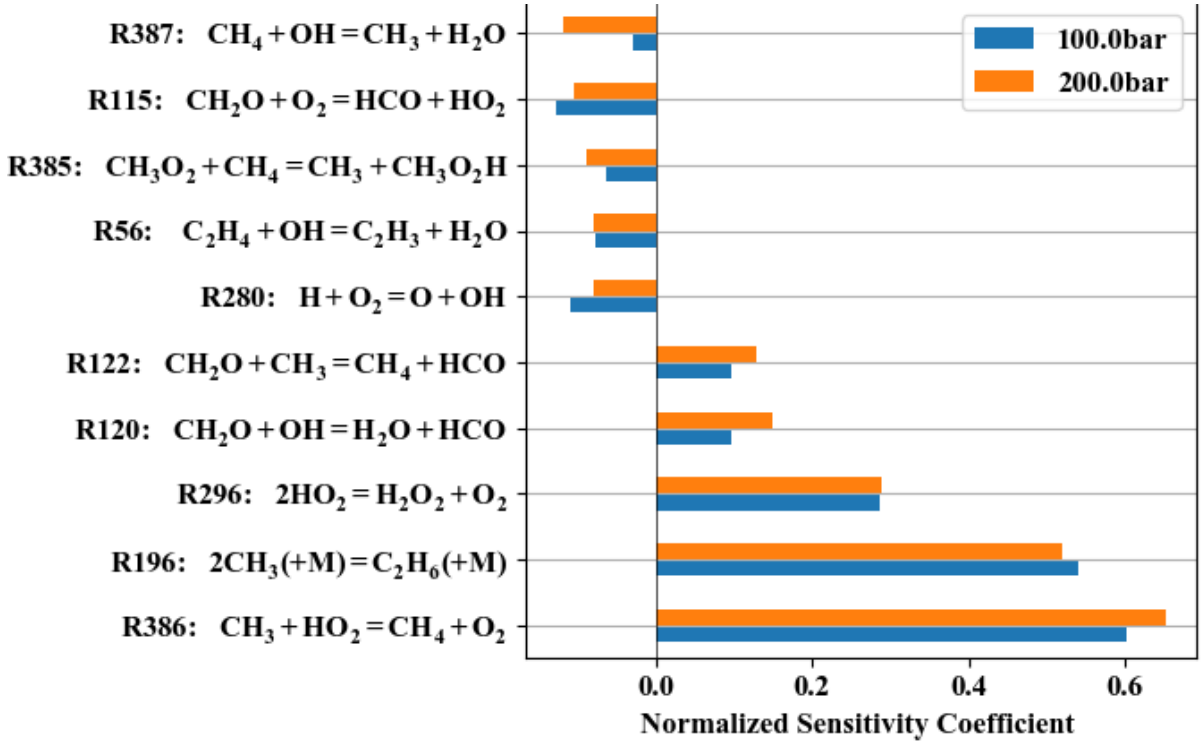


Temperature further distinguishes different kinetic models
- High T kinetics is much simpler than low T kinetics

Chemical Analysis

- $CH_3+CH_3+M=C_2H_6+M$, M should matter
  - It is approaching high pressure limit…
  - How about low pressure?
- The third body efficiency of CO_2 was investigated by doubling its value, which has a negligible effect on autoignition from 1-15 atm

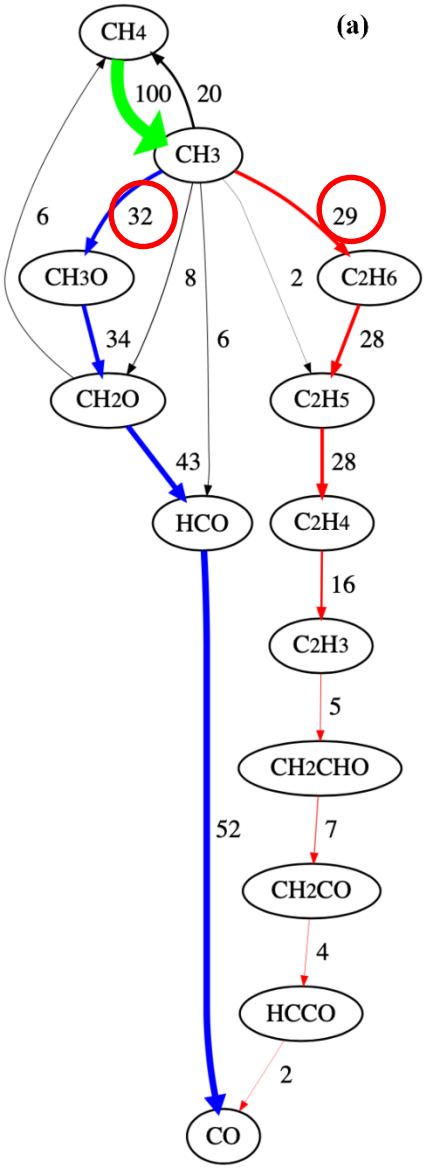
- J.W. Hargis, E.L. Petersen, Energy & Fuels, (29) 2015
- S. Vasu, D.F. Davidson, R.K. Hanson, Energy & Fuels, (25) 2011



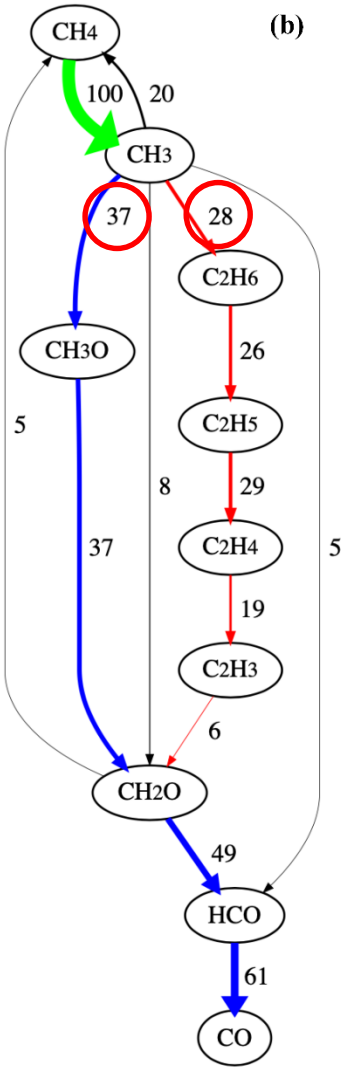
T=1200 K
$CH_4/O_2/CO_2$ mixture
(5:10:85)

CH_4 Reaction Pathway Analysis

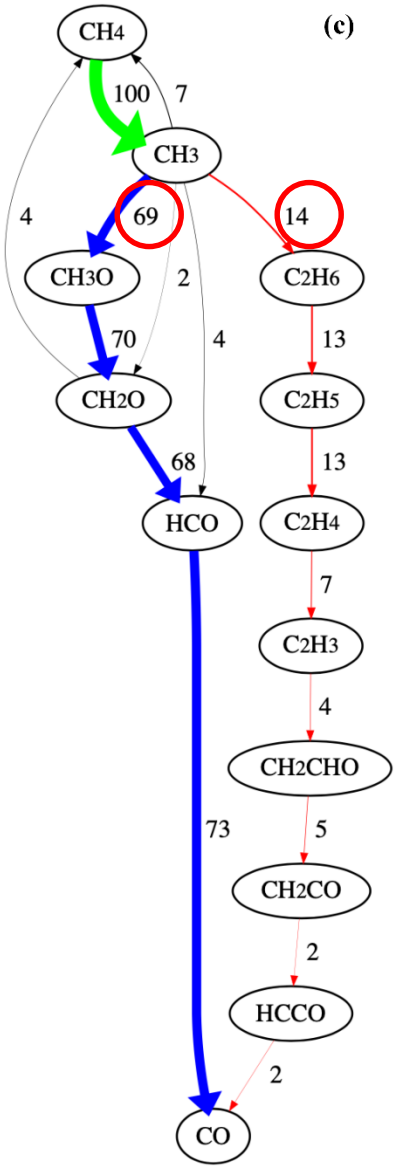
Aramco 2.0



FFCM-1



GRI 3.0

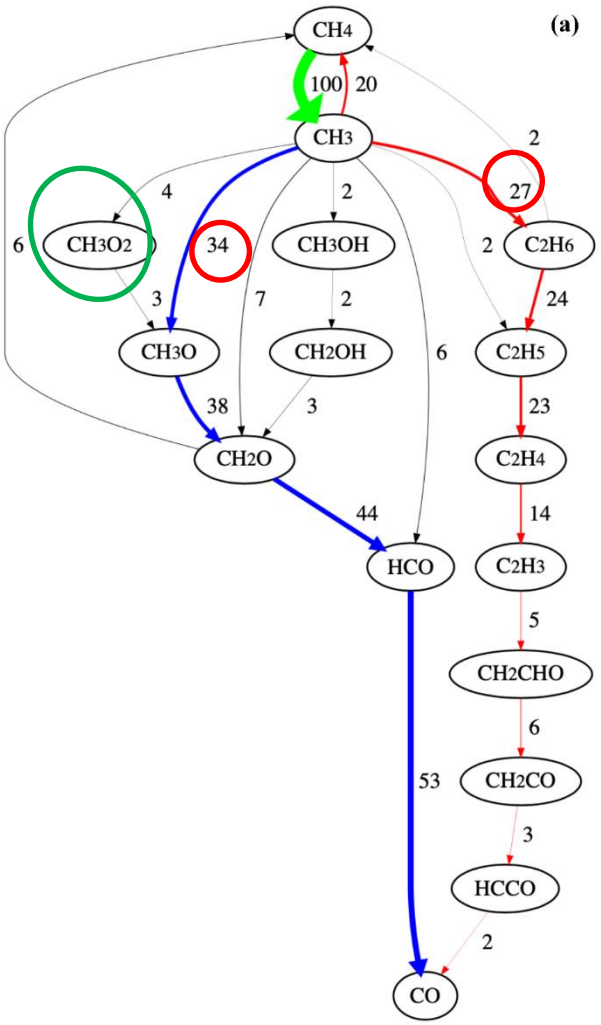


P=100 bar, T=1200 K
$CH_4/O_2/CO_2$ (5:10:85)

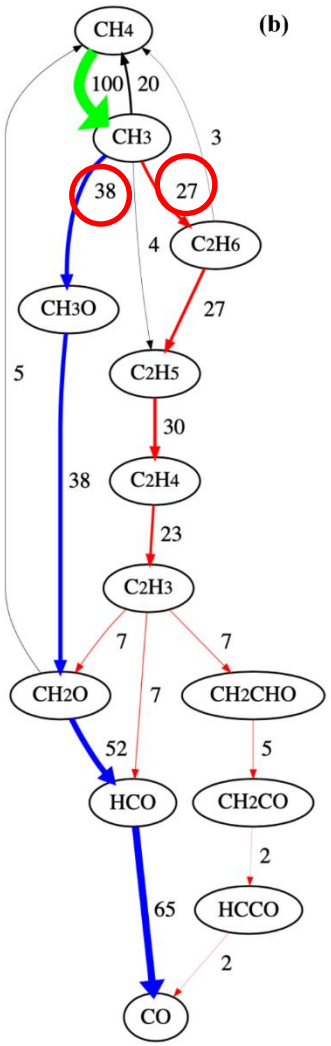
CH_4 branching ratio dictates ignition

CH_4 Reaction Pathway Analysis

Aramco 2.0

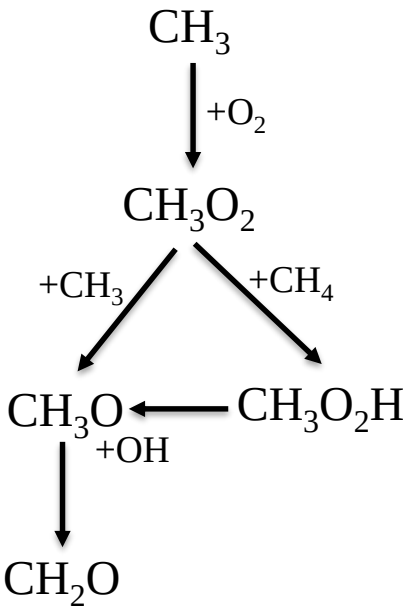


FFCM-1



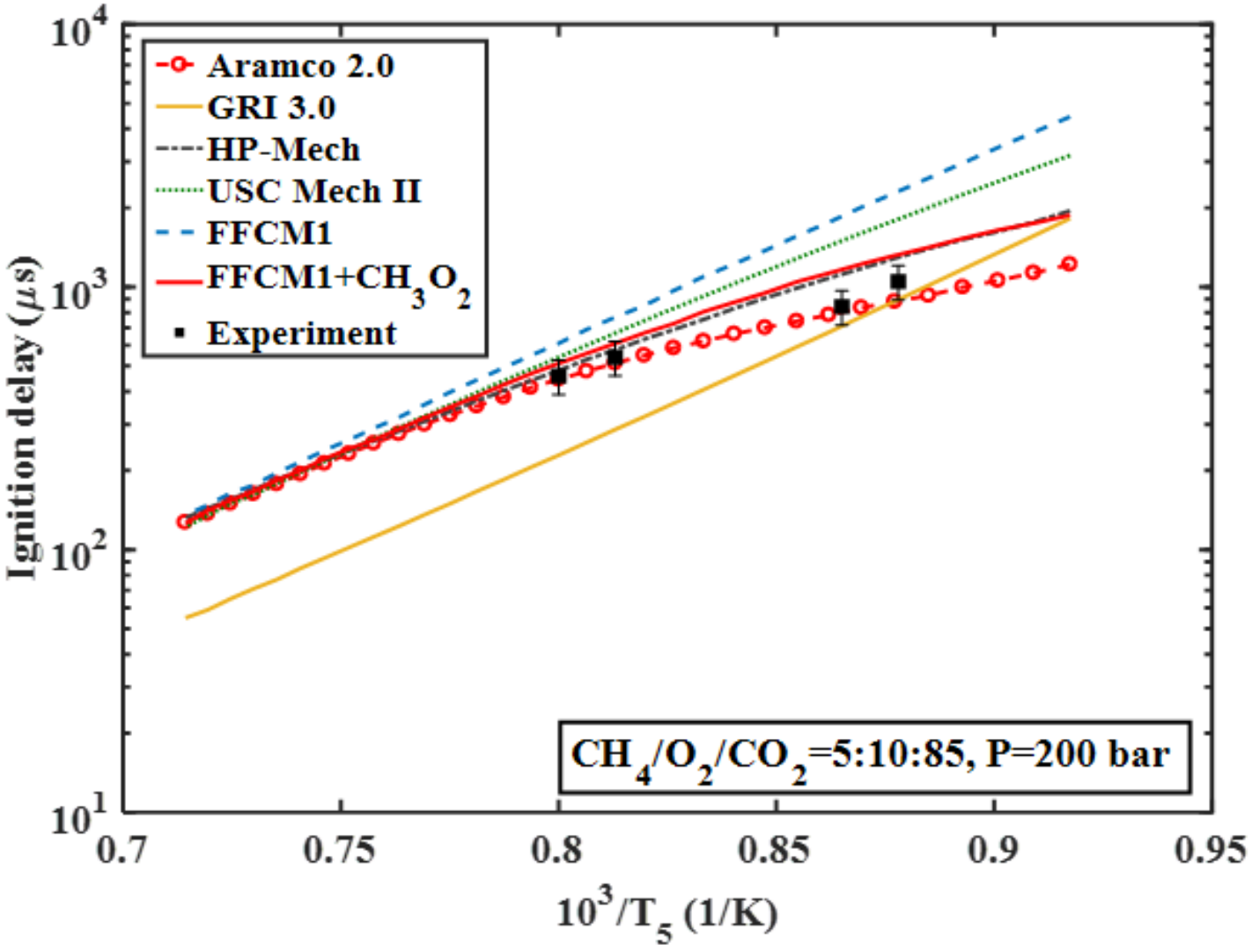
P=200 bar, T=1200 K
$CH_4/O_2/CO_2$ (5:10:85)

Additional pathway of CH_3 at low temperature



CH_3O_2 is NOT included in FFCM

CH_4 Autoignition Delays



Conclusion

- High pressure CH_4 and syngas autoignition delays were measured at 100 and 200 bar
- CH_3O_2 is important at high pressure and relatively low temperature conditions
- CO_2 has chemical effect on elementary reactions through third body collision efficiency, but the overall effect on ignition is washed out

Thank you! & Questions?

Acknowledgement: DoE UTSR Project