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Fundamental Studies to Enable Robust, Reliable, Low Emission Gas Turbine Combustion of High Hydrogen Content Fuels: experimental and computational studies

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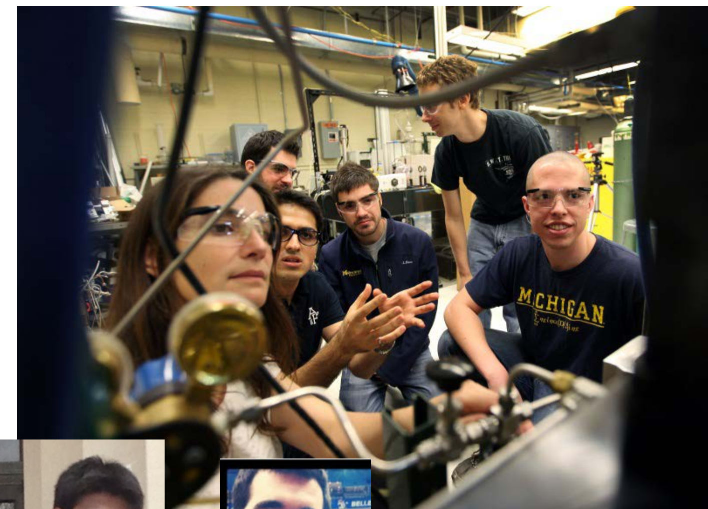
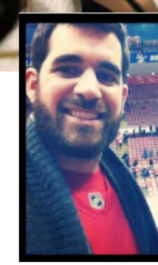
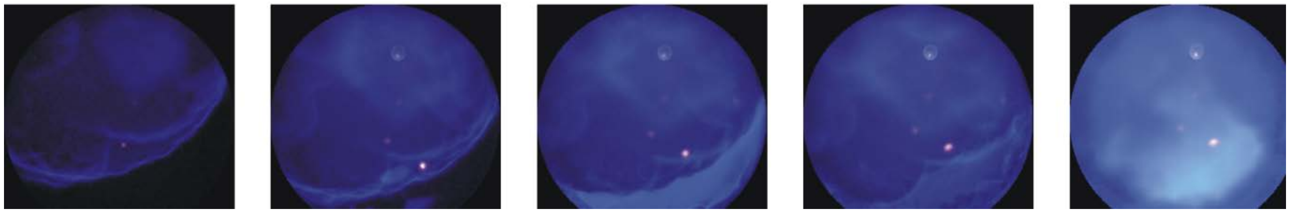
UTSR
University Turbine Systems Research





Many thanks to our UM team and the DOE NETL program!

outline



- *Program objectives*
- *Computational results*
- *Experimental results*

Program objectives

The proposed research program focuses on three areas to advance syngas turbine design:

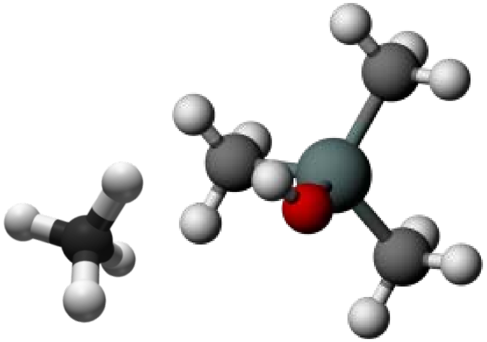
1. syngas chemistry
2. fundamental ignition and extinction limits of syngas fuels
3. data distillation for rapid transfer of knowledge to gas turbine design.

The project objectives are:

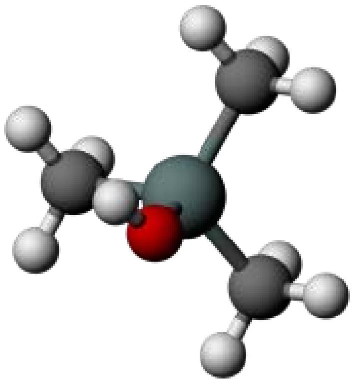
1. **To develop and validate accurate and rigorous experimental and computational data bases of syngas reaction kinetic and fundamental combustion properties**,
2. To develop detailed and reduced syngas chemical mechanisms that accurately reproduce the new experimental data as well as data in the literature,
3. To develop a quantitative understanding of the stability of syngas combustion to fluctuations in the flow field, including the opportunities and challenges of exhaust gas recirculation (EGR) on extinction, ignition and flame stability,
4. **To develop domain maps which identify the range of conditions (e.g. temperature stratification, turbulence, etc.) where syngas combustion can be effected in both positive and negative manners (e.g. accelerated autoignition).**

Projects

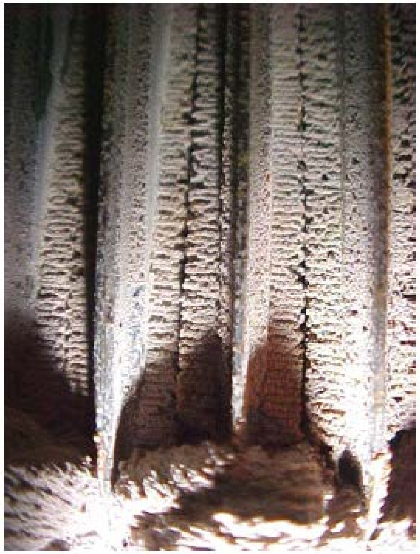
1. Predicting ignition regimes
    1. 1D numerical simulations → Sankaran criterion
    2. Including turbulence → Damkohler criterion
    3. 2D DNS validation
2. Syngas kinetics and the effects of impurities on syngas combustion



The effects of impurities on syngas combustion

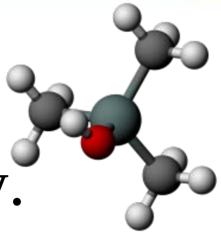


- Numerous impurities in real syngas, with significant impacts on reactivity [15-21]
- Particular concern for **organosilicon compounds**
  - Silanols, siloxanes (like trimethylsilanol) increasing in concentration in landfill-based syngas [13]
  - Known to foul; effects on combustion?
  - SiH_4 has marked effect on H_2, likely also the case for syngas [25, 28]



[Pierce, 2005]

Project Objectives and Approach



1. Syngas kinetics for baseline understanding
2. Effect of trimethylsilanol (**TMS**) on syngas reactivity.
   – Unstudied impurity related to commonly found Si-species in landfill-based syngas

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- Compare ignition times to predictions from typical modeling
- Use model to interpret and analyze observations

P ~ 5 & 15 atm, T ~ 1010 – 1110 K

φ = 0.1, ~Air Dil. with N_2 (CO_2, Ar)

(1) syngas: 30% H_2, 70% CO

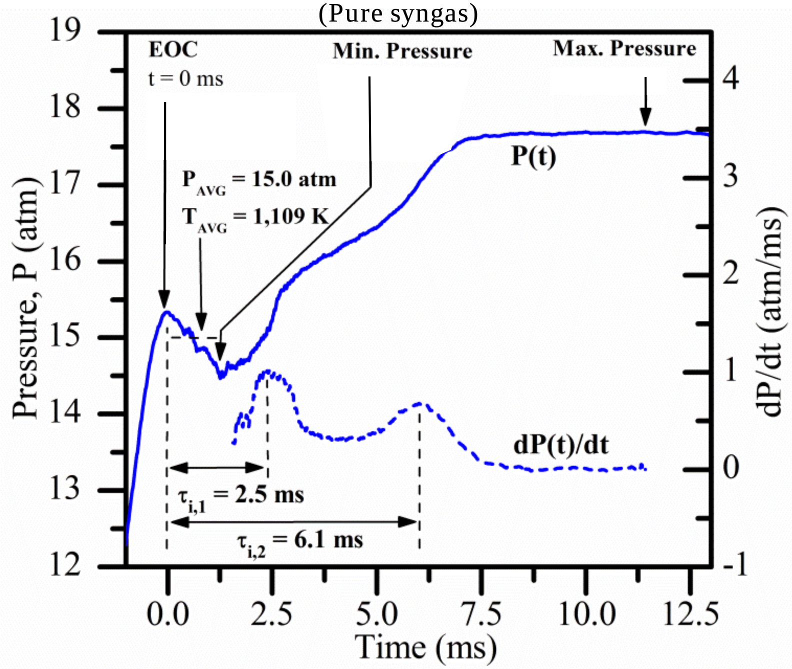
(2) syngas + 10ppm TMS

(3) syngas + 100ppm TMS

Results: Typical Pressure Time Histories during syngas ignition

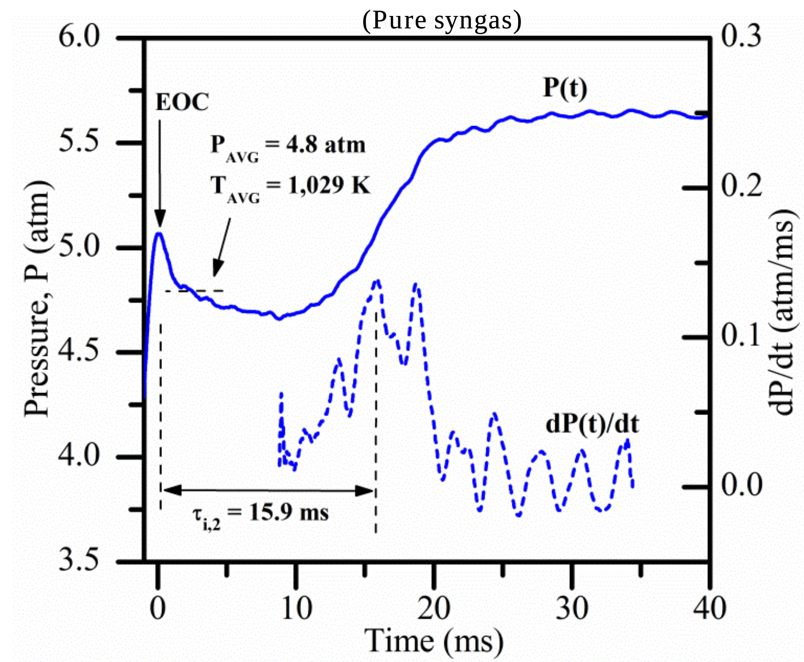
15 atm

Two-step ignition



5 atm

One-step ignition

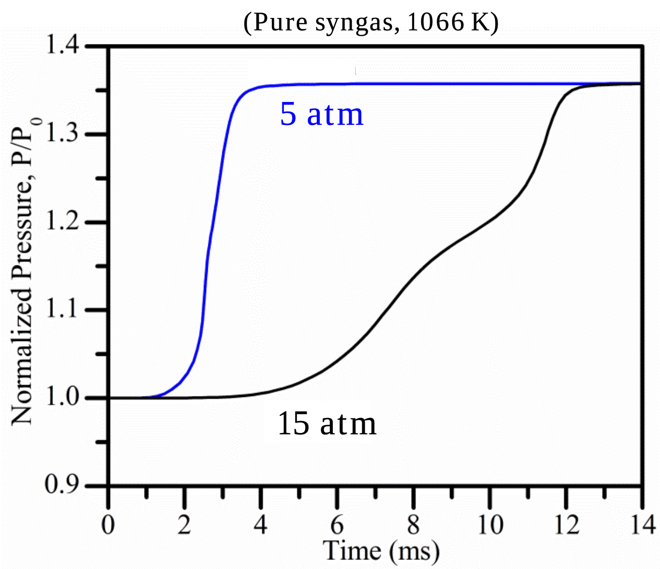


- 2-step ignition never before reported
- Modeling trends indicate worse for higher P, more CO

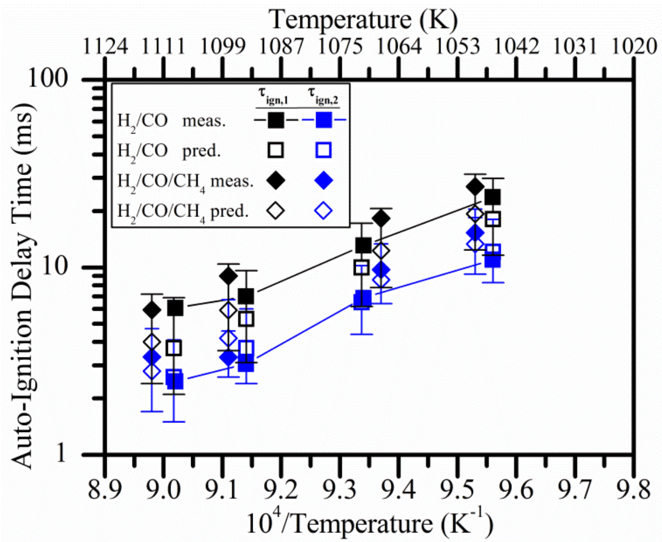
- For each experiment, assigned:
  - Thermo. State (**P**,**T**) , $\tau_{ign, 2}$ and $\tau_{ign, 1}$ (if 2-step)
  - Sources of uncertainty: direct meas. and post-processing filters

Comparison between measurements and model predictions

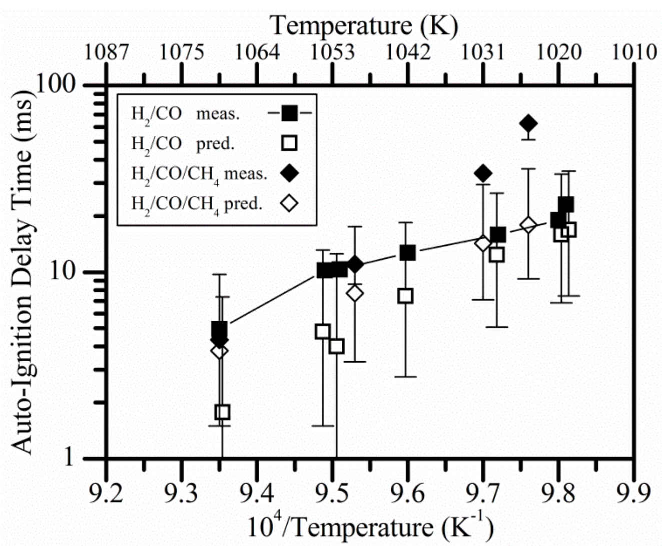
Predicted P-t history



15 atm



5 atm



- Modeling accurately predicts 2-step ignition at 15 atm, 1-step 5 atm
- $\tau_{ign,1\,\&\,2}$ **predictions in excellent agreement** for both P, syn. & syn. + CH_4
- System well represented by Li 2007 mech. and CHEMKIN homog. reactor model

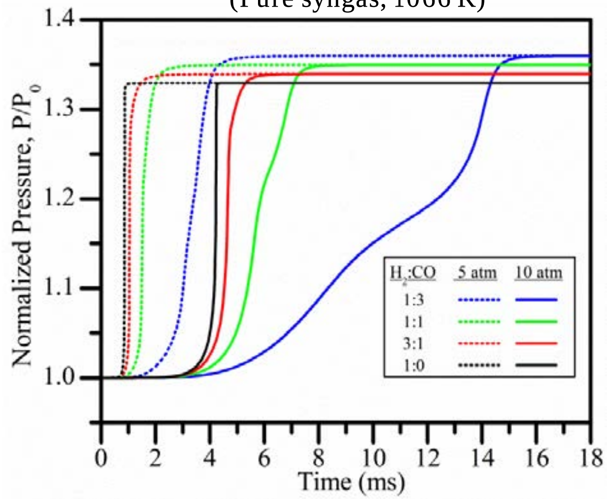
- J. Li, Z. Zhao, A. Kazakov, M. Chaos, F.L. Dryer, and J.J. Scire, A comprehensive kinetic mechanism for CO, CH2O and CH3OH combustion, Int. J. Chem. Kinet. 39 (2007), pp. 109– 136.

combustion LABORATORY

Discussion: Why 2-step Ignition?

Predicted P-t trends

(Pure syngas, 1066 K)



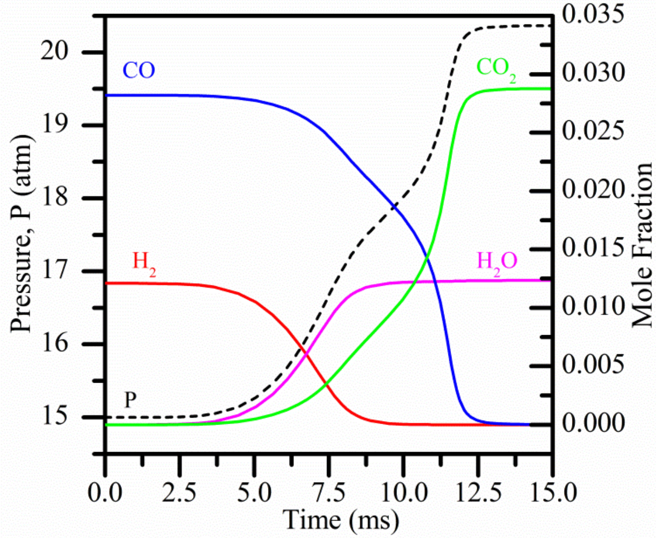
- 2-step behavior minimal at 5 atm, pronounced at 15 atm for high χ_{CO}

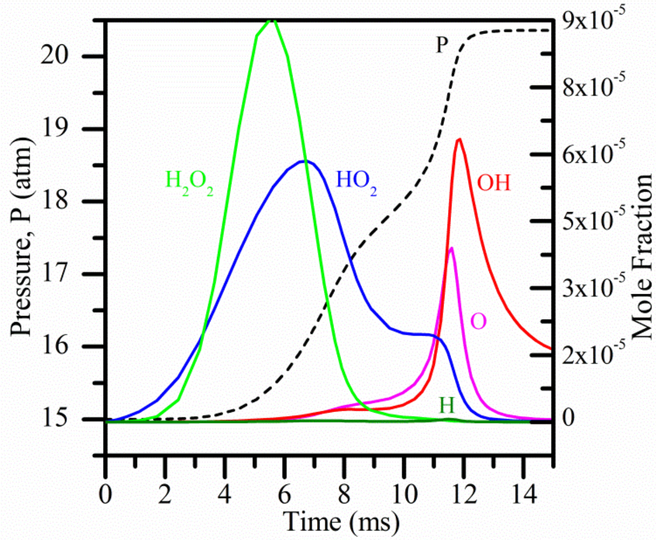
Why 2-step ignition?

(ROP and sensitivity analysis)

- $CO + OH = CO_2 + H$ dominates
- OH lag after step 1, H_2 exhausted
- $H + O_2 = OH + O$ v. $H + O_2(+M) = HO_2(+M)$
- Explains P and H_2:CO (T_{step1}) dependence

Predicted χ_i-t history

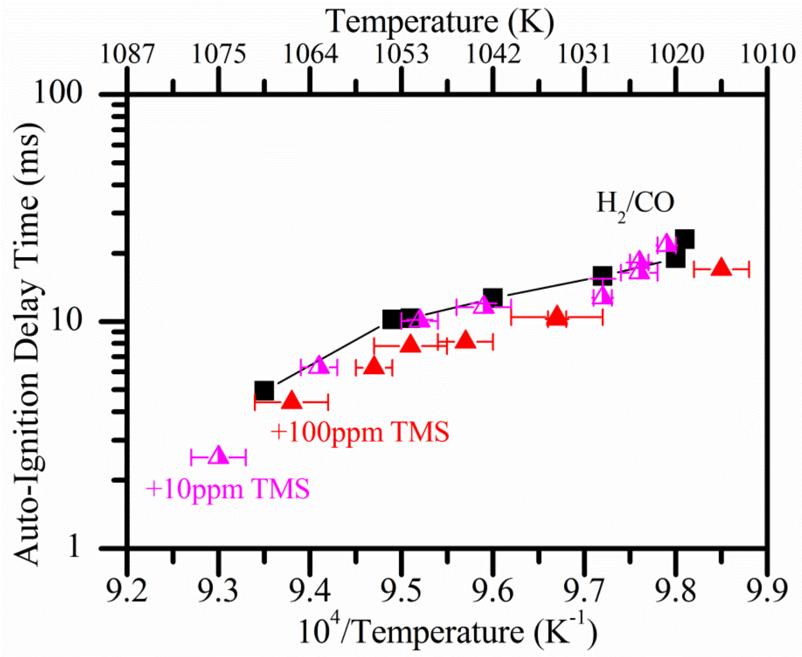




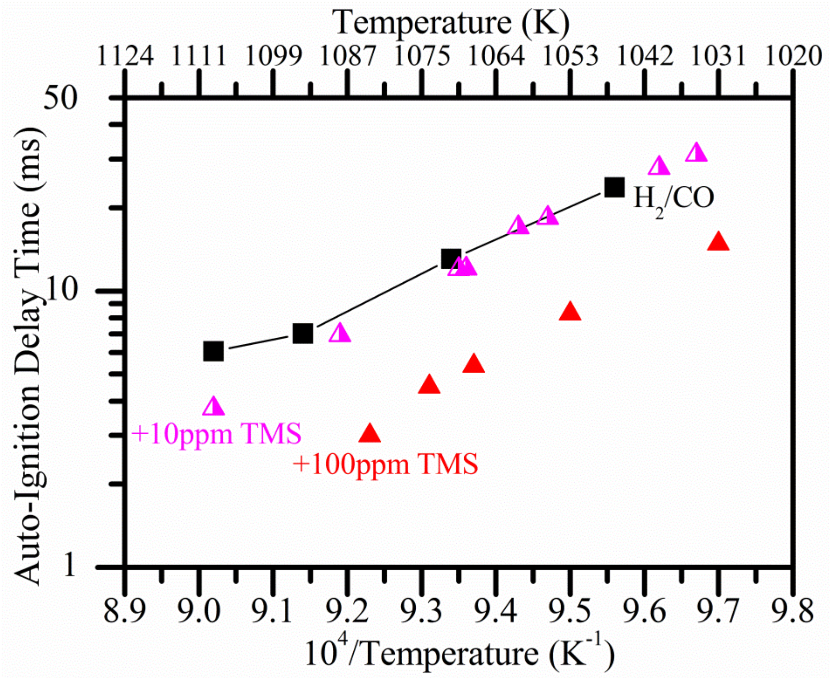
(Pure syngas, 15 atm, 1066 K)

Results: Effects of TMS on τ_{ign}

5 atm



15 atm



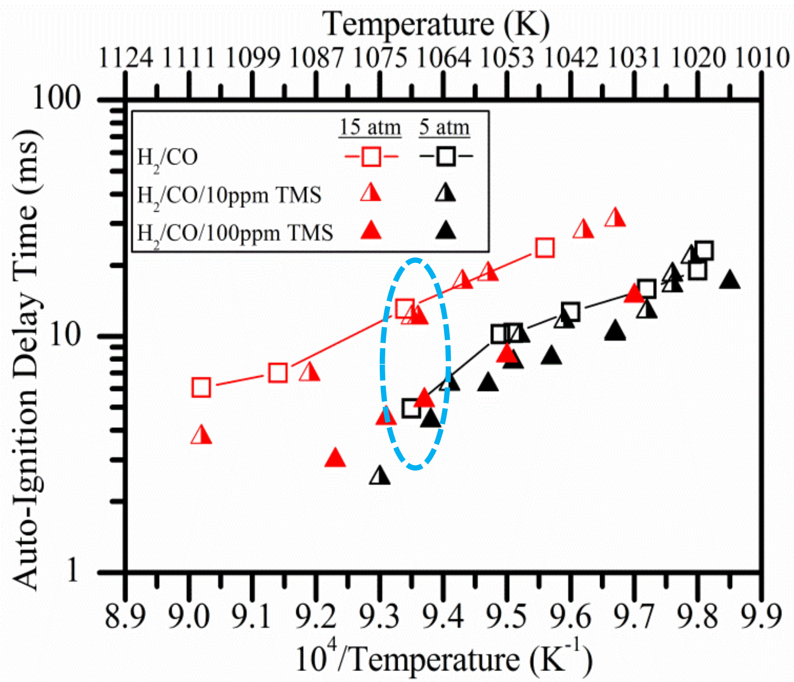
- 10 ppm TMS ~ negligible
- 100ppm TMS decrease by ~**20-30%**

- 10 ppm TMS ~ negligible?
- 100ppm TMS decrease by ~**50-70%**

➢ TMS effect consistent and drastically promoting at 100 ppm!

Results: TMS and P Dependence

$\tau_{ign,2}$



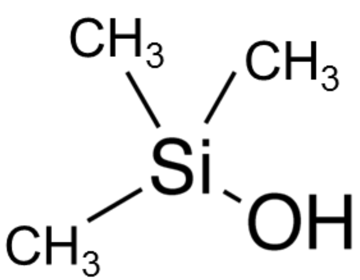
- 100 ppm TMS virtually eliminates P dependence
- Suggests TMS effect is on HO_2/ H_2O_2 chemistry: supported by modeling
- Very similar effects seen for another Si compound, SiH_4 , in H_2 [petersen][mclain]

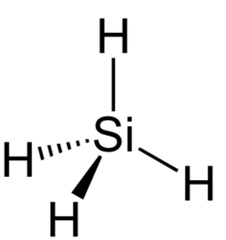
<u>Syngas</u>

- 5 to 15 atm → ~ 100% increase in $\tau_{i,2}$

<u>Syngas + 100ppm TMS</u>

- 5 to 15 atm → ~ negligible increase



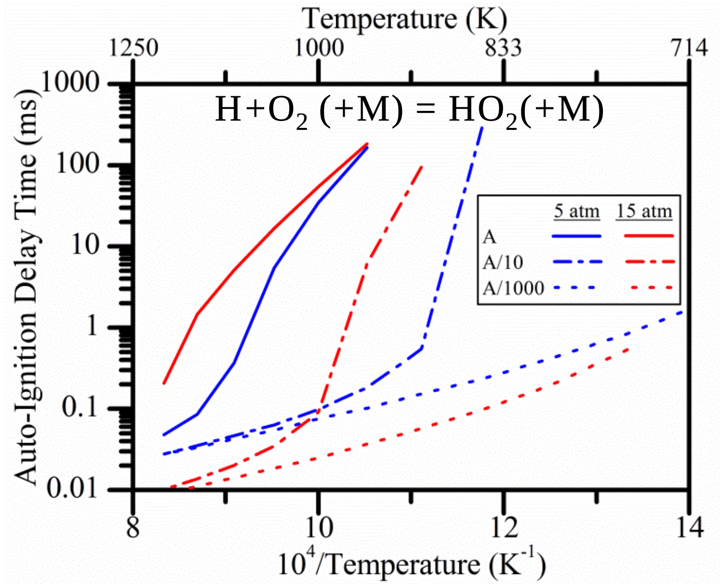


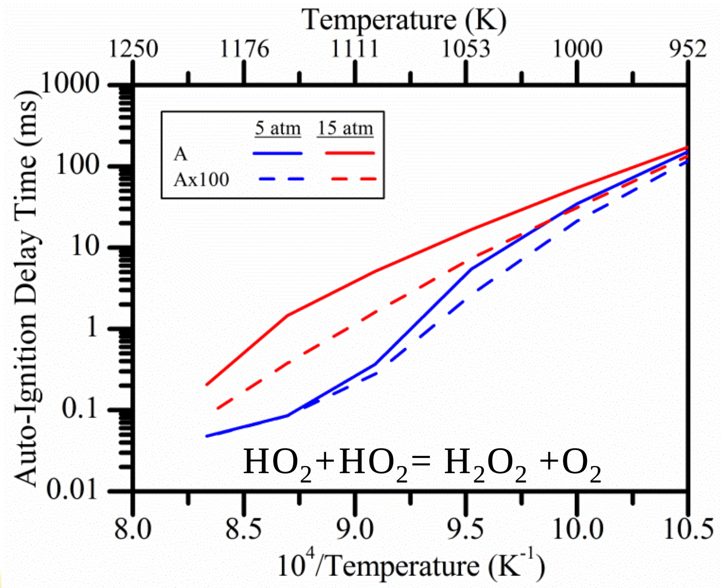
Molecule images:
http://en.wikipedia.org/wiki/

Discussion: Why does TMS have a promoting effect?

- Can't investigate directly using modeling, there are no reaction mechanisms to support the chemistry
- Jachimowski & McLain and Petersen suggested SiH_4 in H_2 disrupts formation and/or enhances consumption **HO_2**
- Simulated these effects using current model with Li 2007 mechanism
    - $H + O_2(+M) = HO_2(+M)$ (A x $10^{1,-1,-3}$)
    - $HO_2 + HO_2 = H_2O_2 + O_2$ (A x $10^{1,-2}$)

- Trends of increased reactivity and lowered pressure dependence replicated, but magnitude of effects are not consistent with experimental observations
- HO_2 interaction likely part of the TMS effect, but not all of the effect





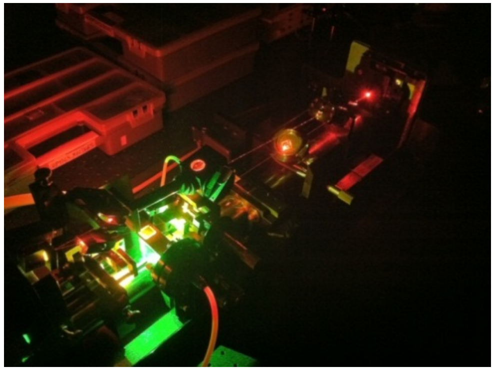
Current work : OH measurements

Goal

Measure $\chi_{OH}(t)$ during syngas auto-ignition.

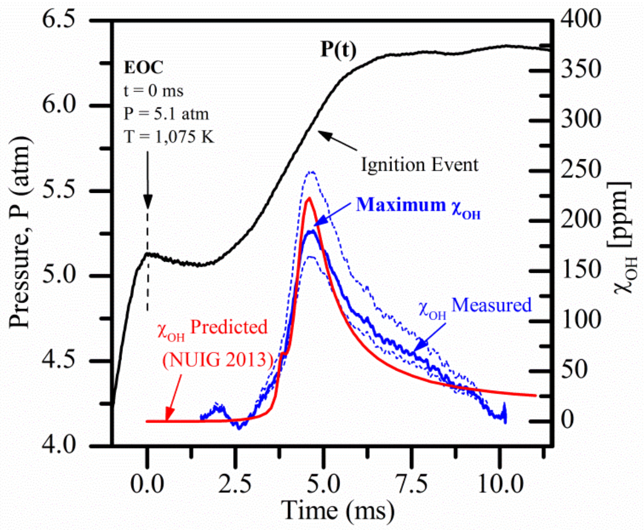
Conditions

P ~ 5 atm, T ~ 1000-1090 K, φ = 0.1, ~Air Dil., N_2 (Ar)
Fuel: 30% H_2, 70% CO, with and without TMS impurities



- Low precision targets dominate (τ_{ign}, s_L^0) available kinetic data
- Important O, OH, H radical data very limited for H_2 (high-T, low-P, ultra dilute) [29], unstudied for syngas

  - Initial results show visible OH absorption feature
  - Excellent agreement between measured and predicted $\chi_{OH}(t)$
  - Interrogation of multiple features possible (magnitudes, slopes), to improve chemical kinetics



Thank you!

Questions/Comments?

$50 Million Renovation of the GG Brown Memorial Laboratories

TOP: Rendering of new stairway connecting public spaces.
BOTTOM: GG Brown during the construction phase.

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