Exploring flameless combustion using thermal steady-state multiplicity in PSRs

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SUPERVISOR

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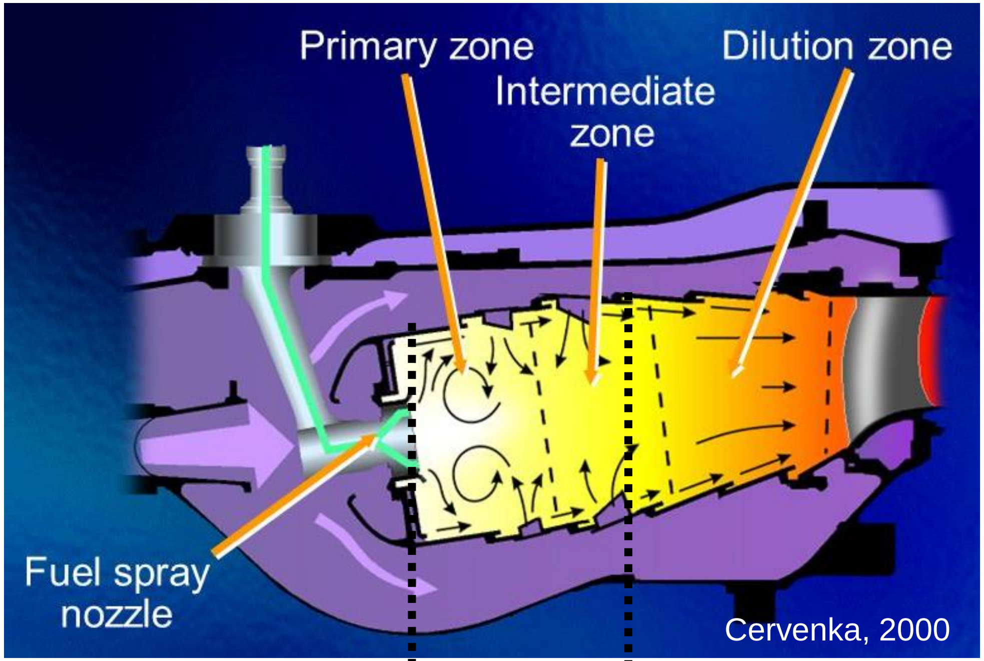
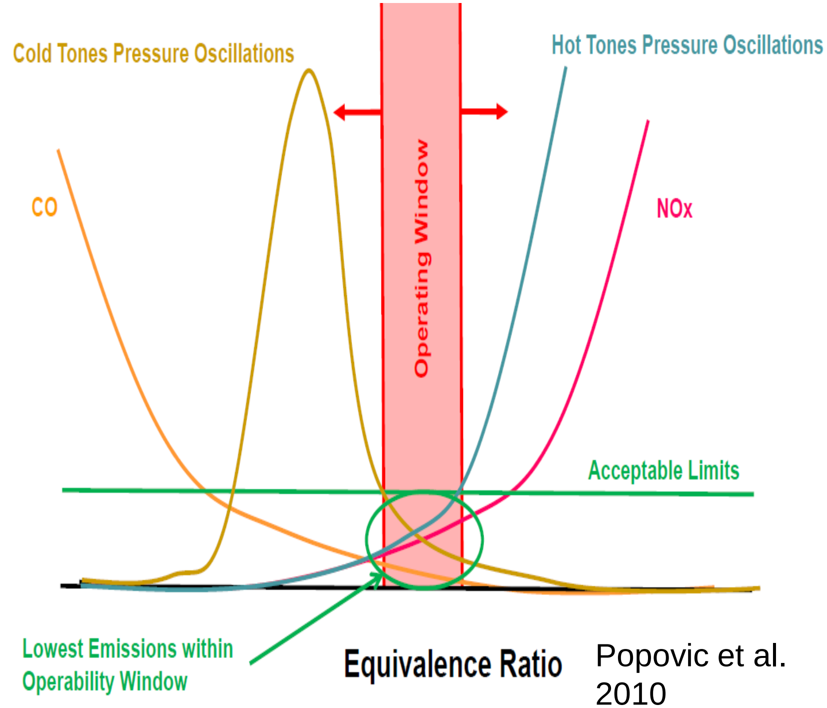
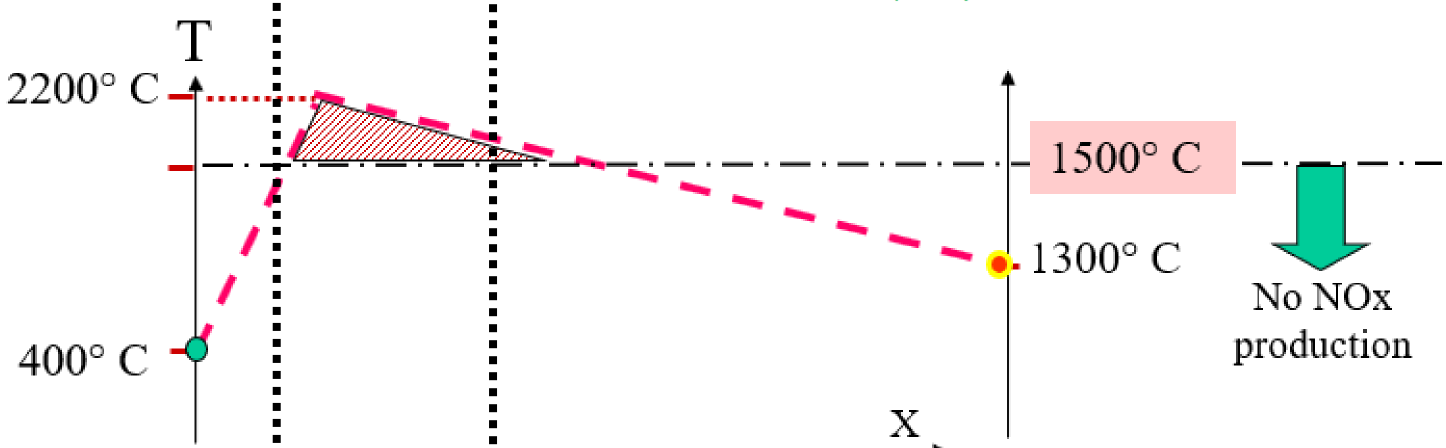
Gas Turbine Combustor Emissions





Popovic et al. 2010



M. Cervenka, "The Rolls-Royce Trent Engine", 2000
Popovic P, Myers G, Citeno J, Symonds R, Campbell A. Fuel Flexibility With Low Emissions in Heavy Duty Industrial Gas Turbines. ASME. Turbo Expo: Power for Land, Sea, and Air, *Volume 2: Combustion, Fuels and Emissions, Parts A and B* ():163-172

Flameless Combustion – Principle

Hydrocarbon + Oxidizer + Inert → Oxidized Reactant Molecules + Inerts

REACTANTS → **PRODUCTS**

Reactants

- Vitiated Environment
- +
- $T_{initial} > T_{autoignition}$

→ **Increased Chemical Timescale** →

Products

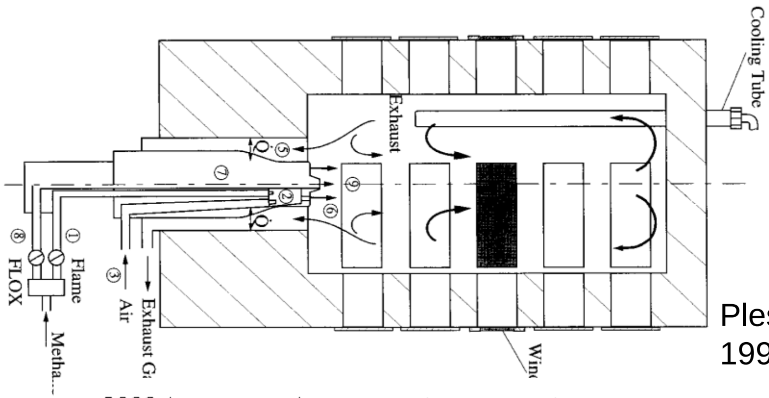
- FLAMELESS COMBUSTION

"Flameless oxidation is stable combustion without a flame and with defined recirculation of hot combustion products." – J. G. Wunning

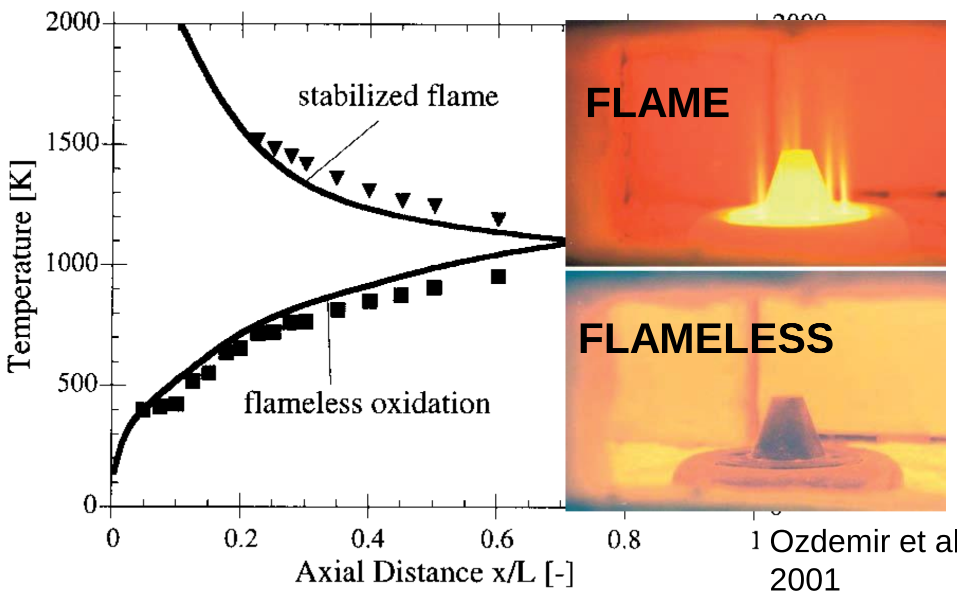
(HTACG-Poland, 2010).

Flameless Combustion - Experimental

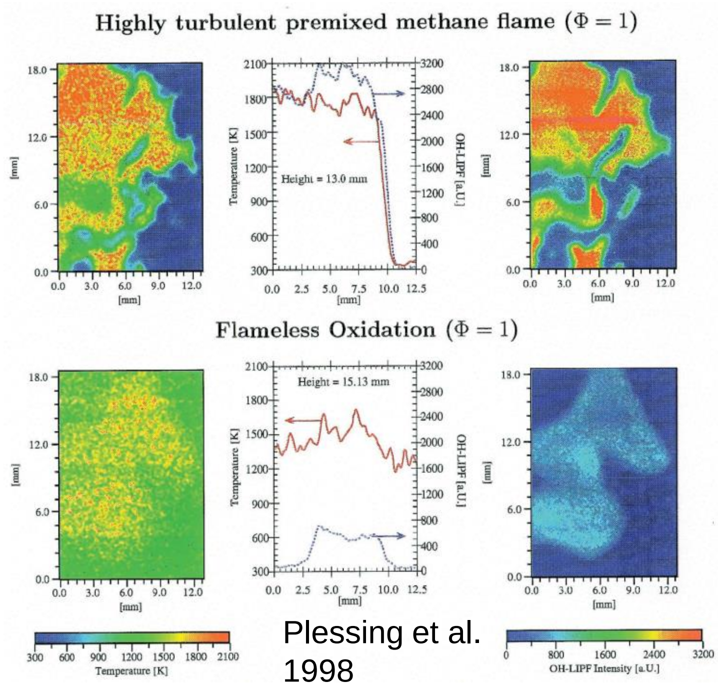
Wunning Type Flameless Burner



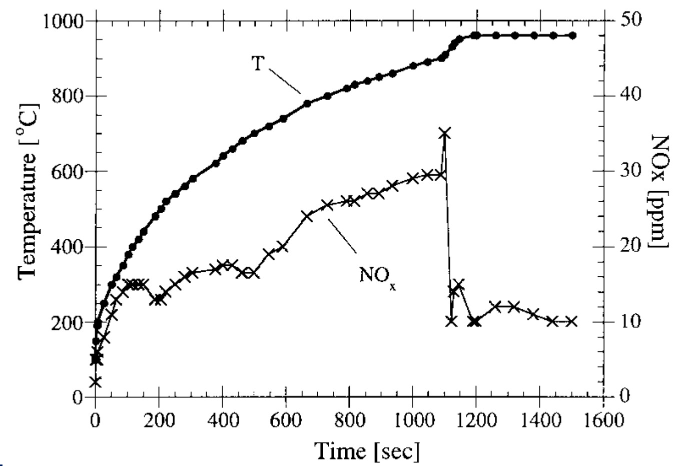
Plessing et al. 1998



Ozdemir et al. 2001



Plessing et al. 1998

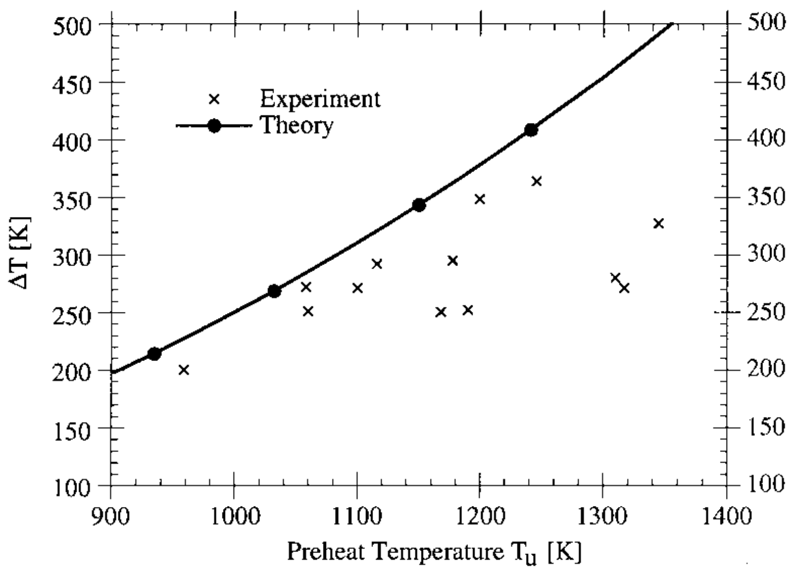


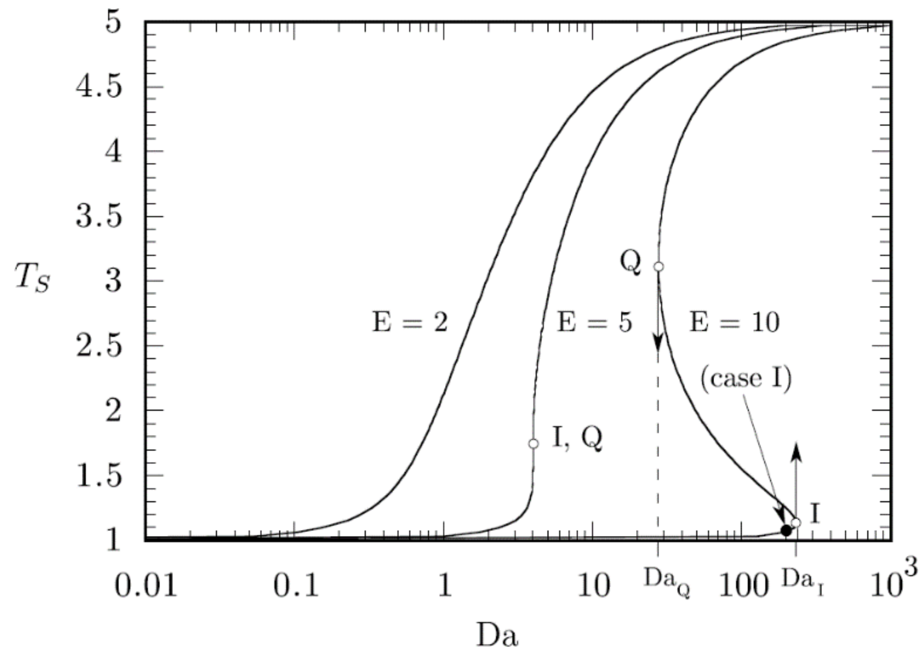
T. Plessing, N. Peters and J. G. Wünning, "Laseroptical investigation of highly preheated combustion with strong exhaust gas recirculation," in *Twenty-Seventh Symposium (International) on Combustion*, 1998.

Methodology

Theoretical Study on Flameless Combustion:

- Through analysis of a PSR steady state mass and energy balance equations.
- Temperature rise used to indicate PSR-like behavior.





Non-dimensional activation energy, $E = E_{act}/RT_u$

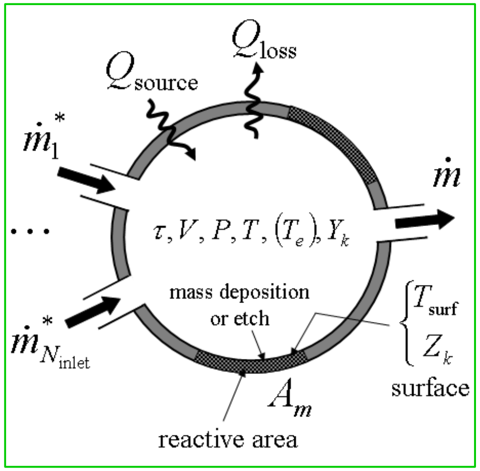
Damköhler number, $Da = \frac{residence\ time}{reaction\ time}$

T. Plessing, N. Peters and J. G. Wünning, "Laseroptical investigation of highly preheated combustion with strong exhaust gas recirculation," in *Twenty-Seventh Symposium (International) on Combustion*, 1998.

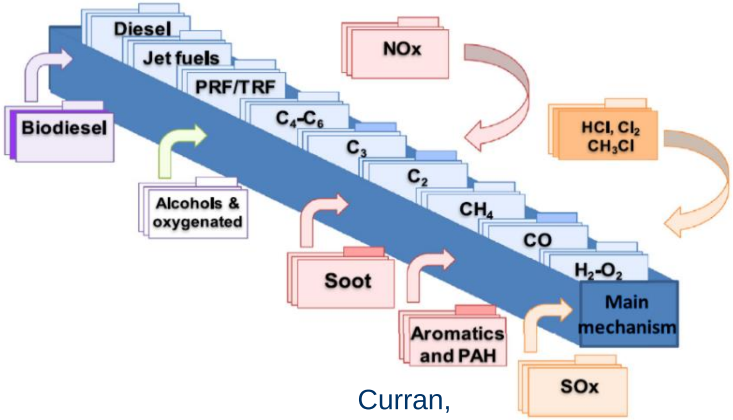
Analysis Tools:

- PSR allows studying the nature of chemical reactions independent of transport characteristics.
- Feedback effects in the system other than diffusional transport effects.
- PSRs allow the study of multiple steady states that can occur in a system for the same set of inlet conditions.
- Multiplicity due to inherent feedback in the system.

PERFECTLY STIRRED REACTOR (PSR)



CHEMICAL KINETIC MECHANISMS



Curran, 2019

H. J. Curran, "Developing detailed chemical kinetic mechanisms for fuel combustion," *Proc. Comb.Instit*, vol. 37, pp. 57-81, 2019.
Kee et al.., Chemkin Collection, Release 3.7, Reaction Design Inc, San Diego, CA, 2002

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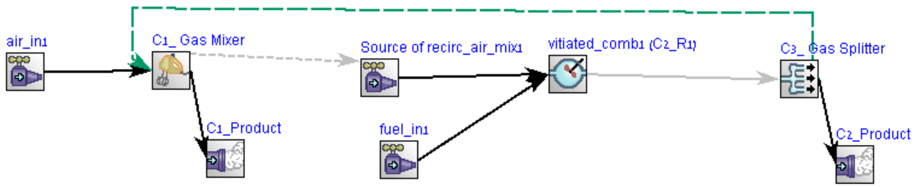
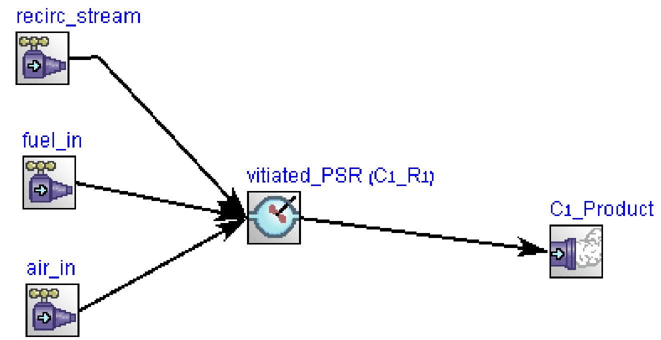
Analysis Tools:

- ANSYS Chemkin used to solve the mass and energy balance equations.
- ARAMCO Mech 3.1 from the University of Galway, Ireland used for modelling the kinectic mechanism of hydrocarbon combustion process.
- Continuation to study the ignition/extinction points carried out using Chemkin – only single parameter continuation allowed.

$$k = \frac{\text{recirculated mass flowrate}}{\text{air flowrate} + \text{fuel flowrate}}$$





<u>Chemical Kinetic Mechanism</u>
AramcoMech3.0 (Zhou et al. 2018)

```
=====================================================================
KINETICS MECHANISM:
   Total number of gas phase species      =  581
   Total number of gas phase reactions    = 3037
=====================================================================
```


C. W. Zhou, et al., *Combustion and Flame*, vol. 197, pp. 423-438, 2018.
Kee et al.., Chemkin Collection, Release 3.7, Reaction Design Inc, San Diego, CA, 2002

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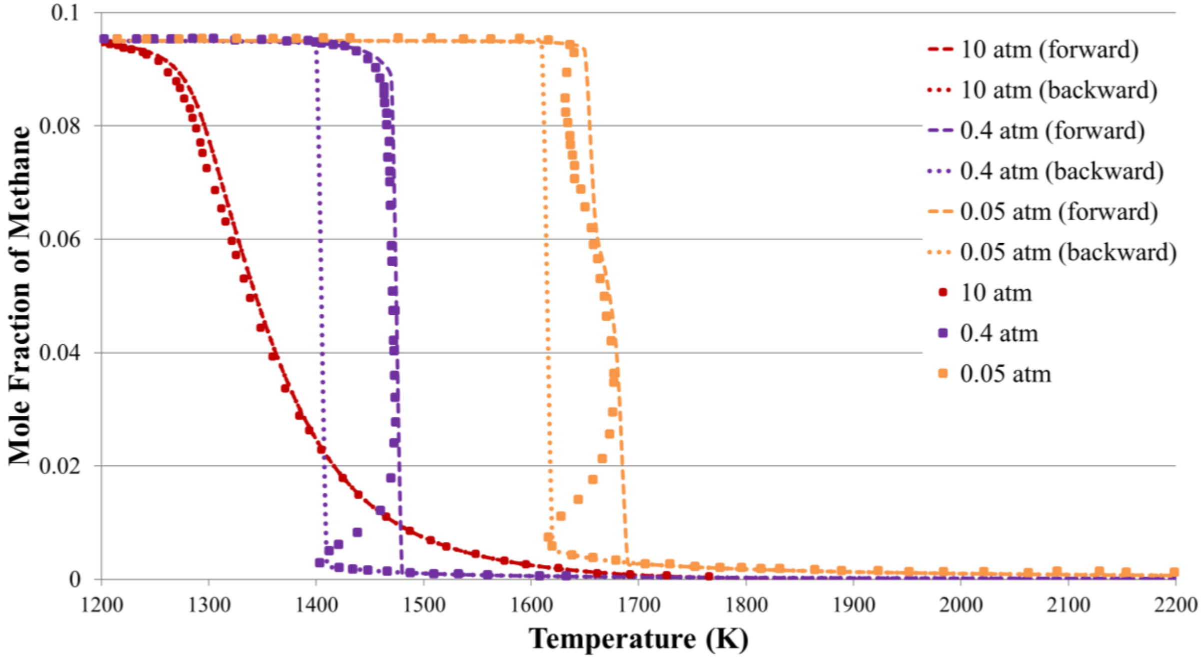
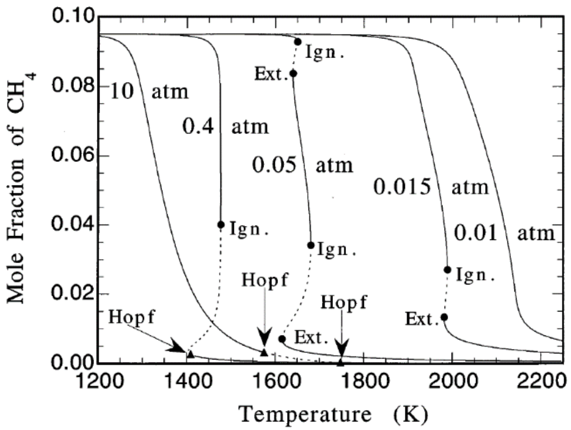
Validation of Chemkin Model:

- Study of Park and Vlachos (1998) used to determine the validity of kinetic model and simulation of transition from multiple steady-state behavior to a unique solution of the balance equations.
- Stoichiometric methane in air reaction (9.5% methane) at 10^{-3} s residence time at different pressures is presented.
- Only the turning points could be determined using Chemkin.
- Mole fraction of methane used to indicate the reaction progress.



Chemical Kinetic Mechanism
GRI Mech 1.2



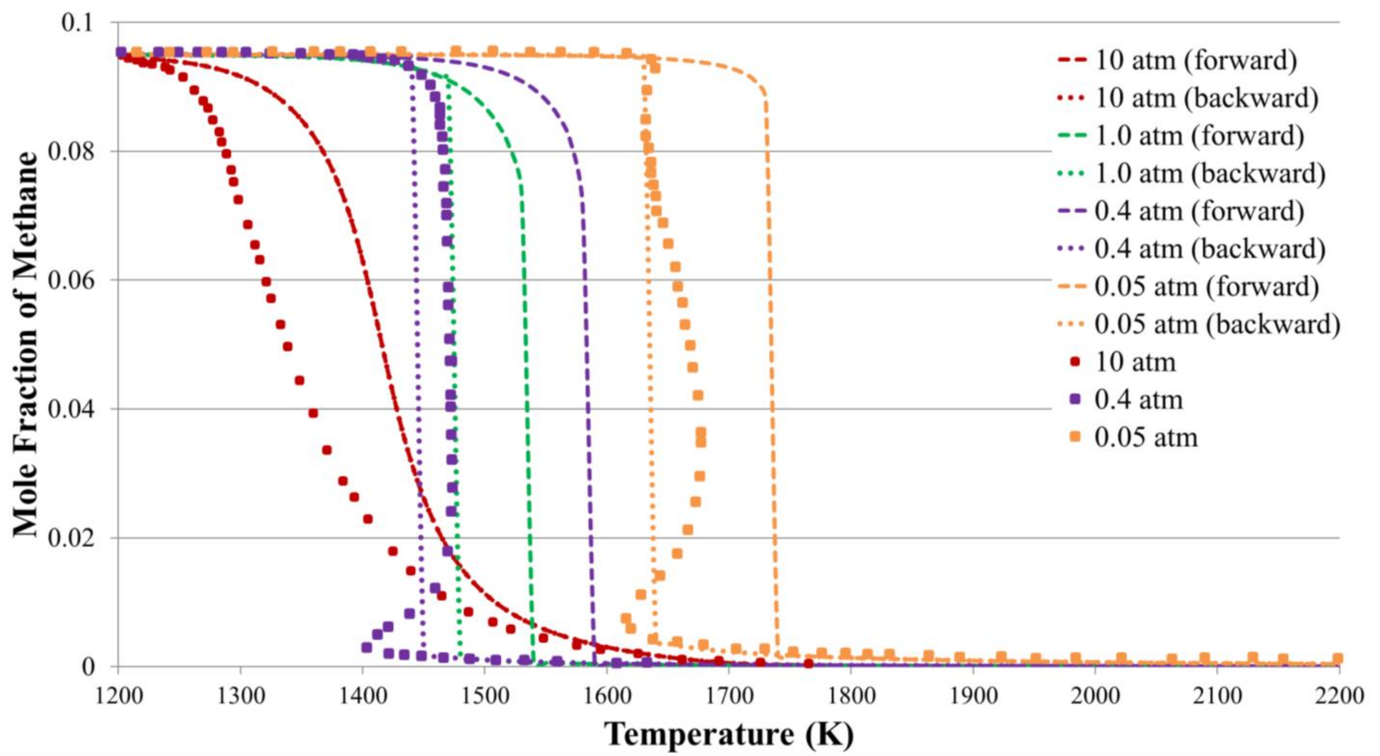
Park & Vlachos, 1998

C. W. Zhou, et al., *Combustion and Flame*, vol. 197, pp. 423-438, 2018.
Kee et al., Chemkin Collection, Release 3.7, Reaction Design Inc, San Diego, CA, 2002

Methodology

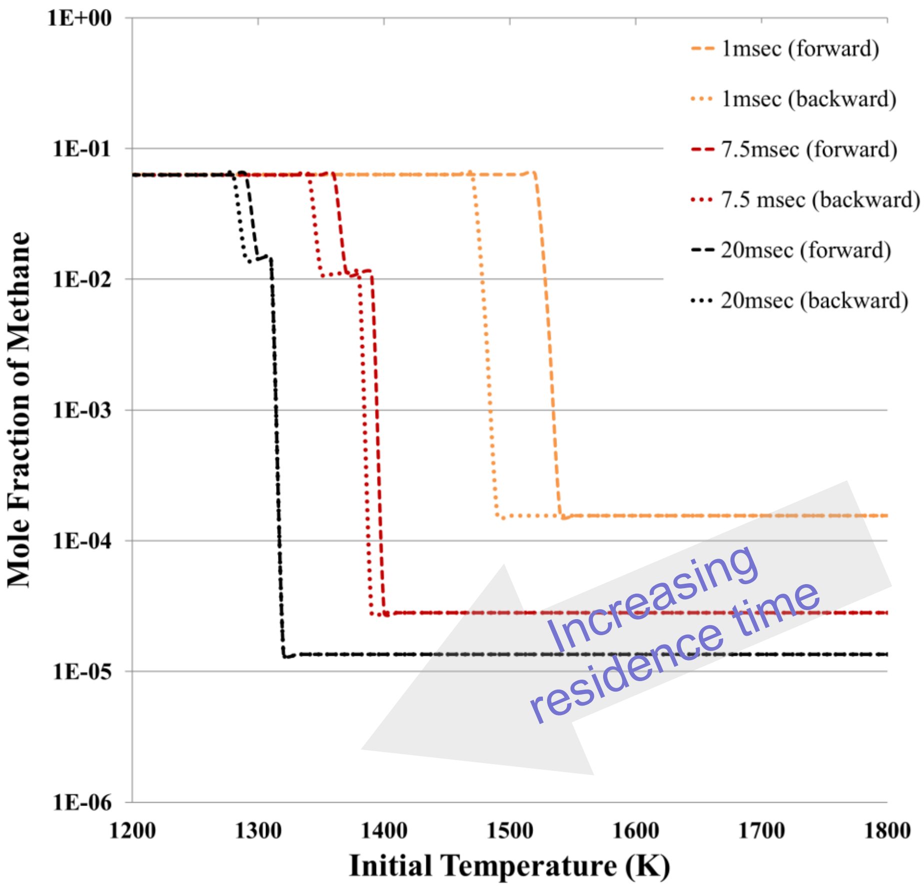
Choice of Chemical Kinetic Mechanism

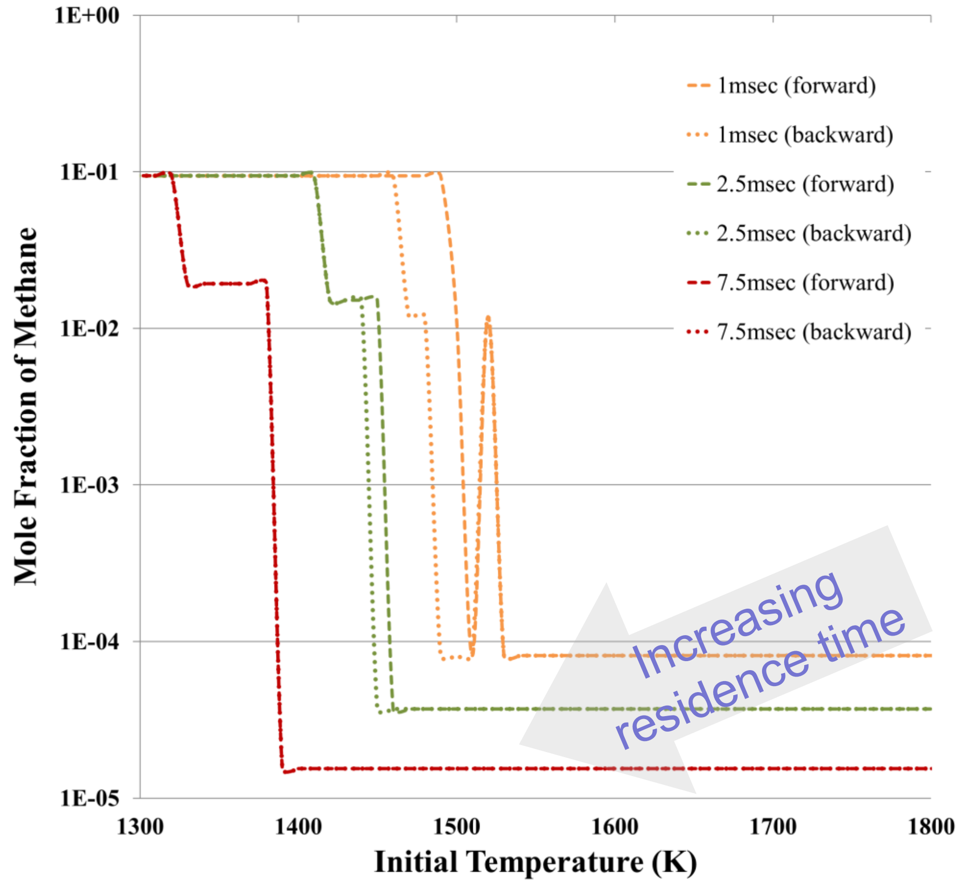
- C1-C4 Hydrocarbon combustion model – **AramcoMech3.0** (Zhou et al. 2018)
- Most accurate methane combustion kinetic mechanism for a wide range of operating conditions (O.Mathieu et al., 2019)
- Study can be extended to fuels other than methane.



C. W. Zhou, et al., *Combustion and Flame*, vol. 197, pp. 423-438, 2018.
O.Mathieu et al., *Fuel*, vol 236, pp 1164-1180, 2019.

Results - Variation of Mole Fraction of Methane with Residence Time (Constant Mass Flowrate)

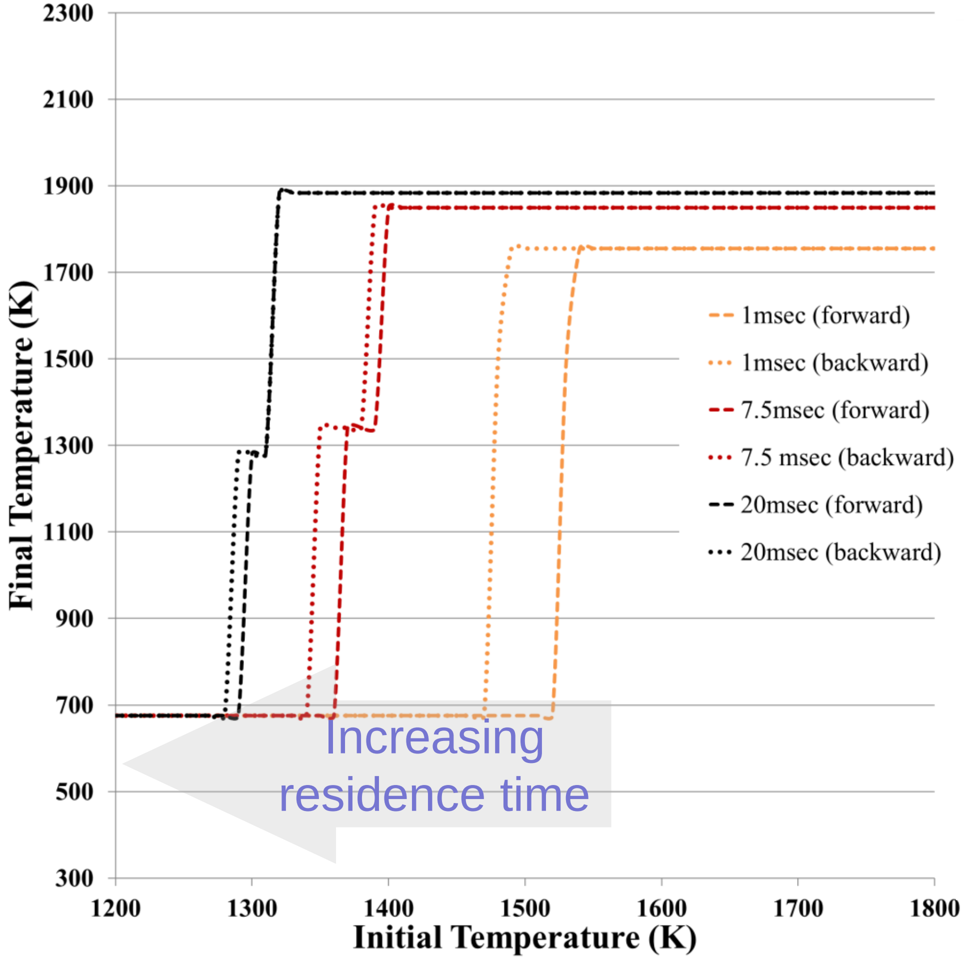




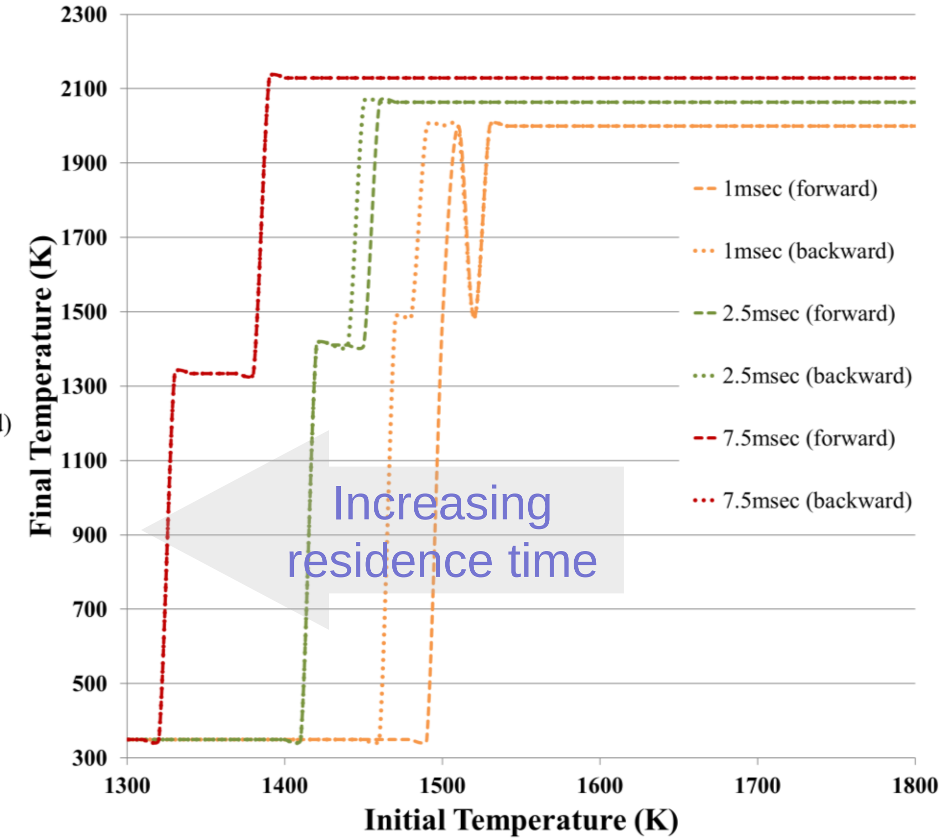
Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0.5 ; Recirculated Stream Temperature = 1250 K

Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0

Results - Variation of Final PSR Temperature with Residence Time (Constant Mass Flowrate)



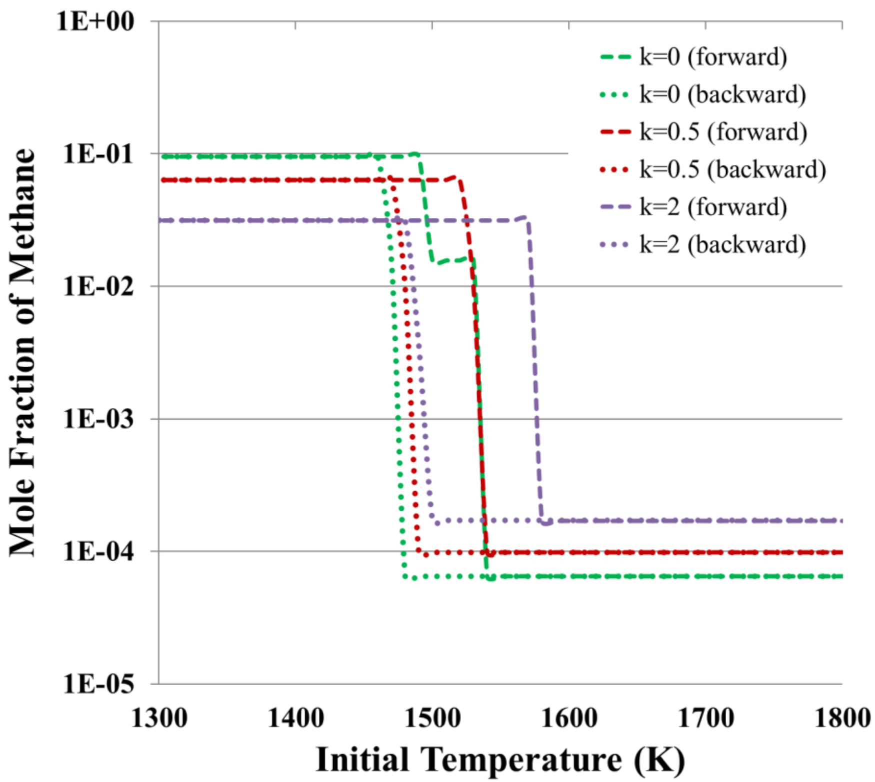
Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0.5 ; Recirculated Stream Temperature = 1250 K



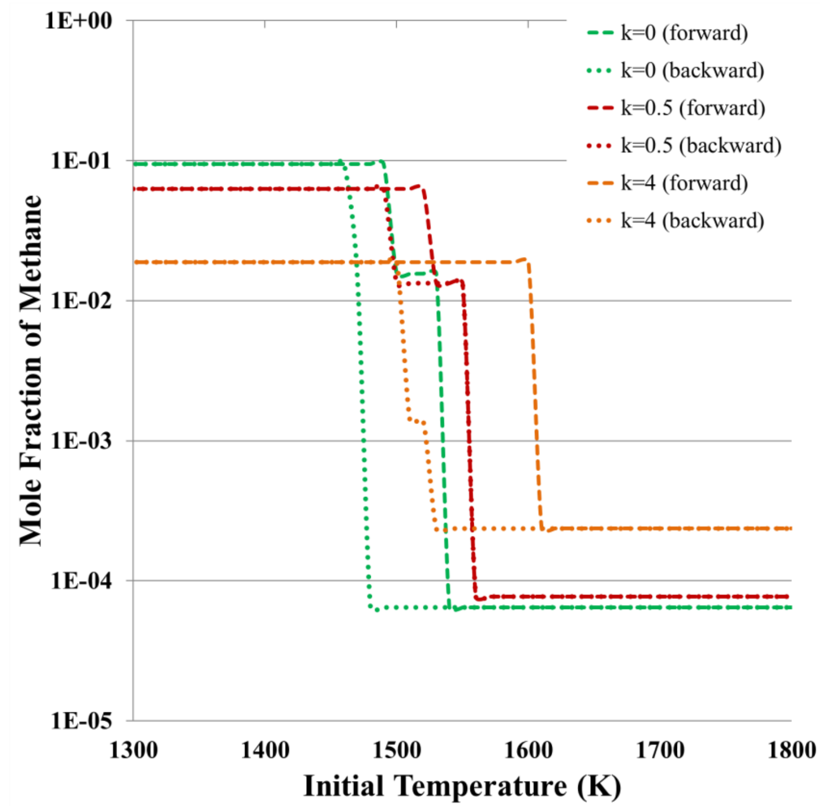
Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0

Results - Variation of Mole Fraction of Methane with Recirculation Ratio

Air Inlet Temperature = 500 K; Fuel Inlet Temperature = 500 K; Recirculated Stream Inlet Temperature = 1500 K



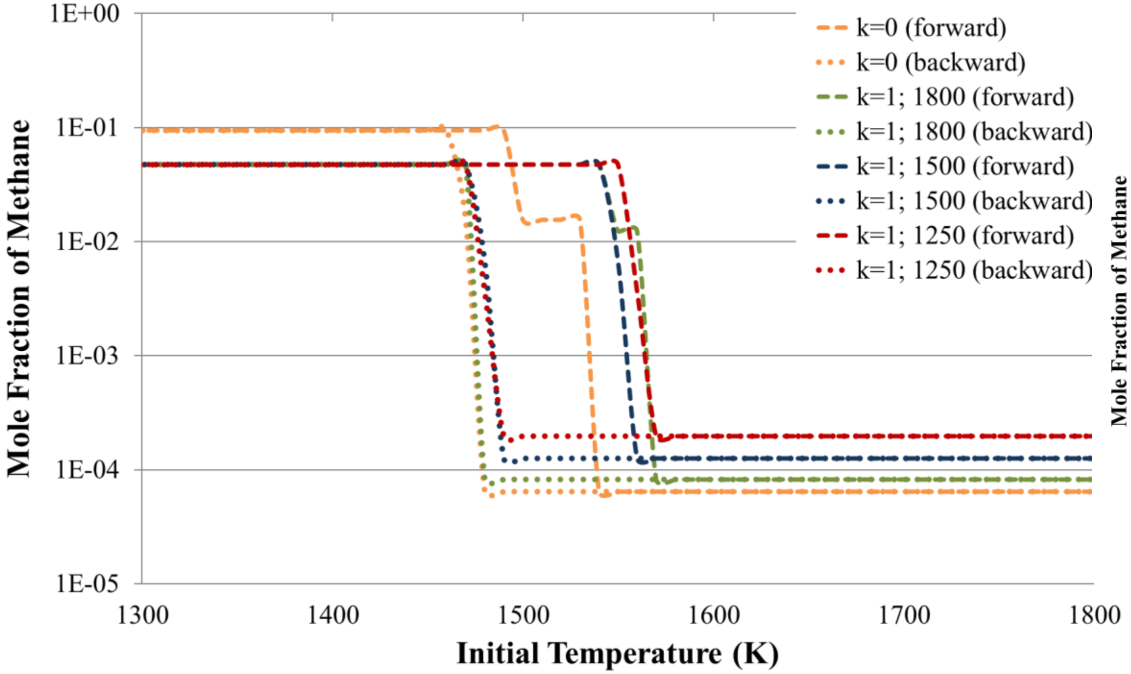
Air Inlet Temperature = 500 K; Fuel Inlet Temperature = 500 K; Recirculated Stream Inlet Temperature = 1500 K



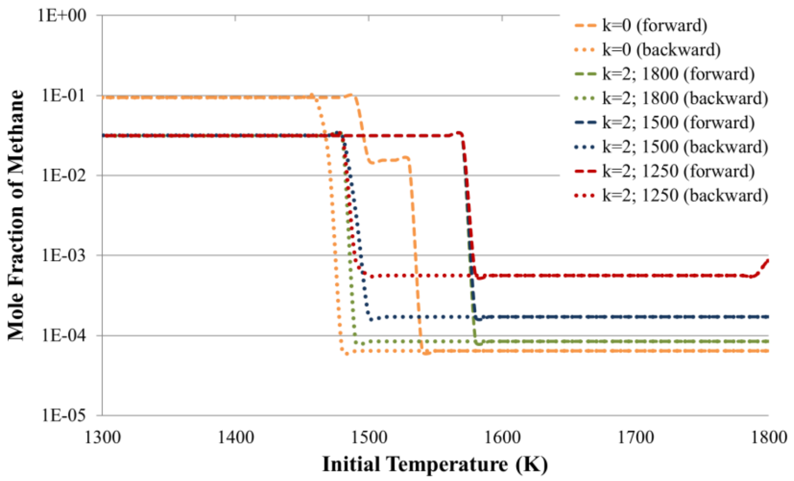
$$k = \frac{\text{recirculated mass flowrate}}{\text{air flowrate} + \text{fuel flowrate}}$$

Results - Variation of Mole Fraction of Methane with Recirculated Stream Temperature

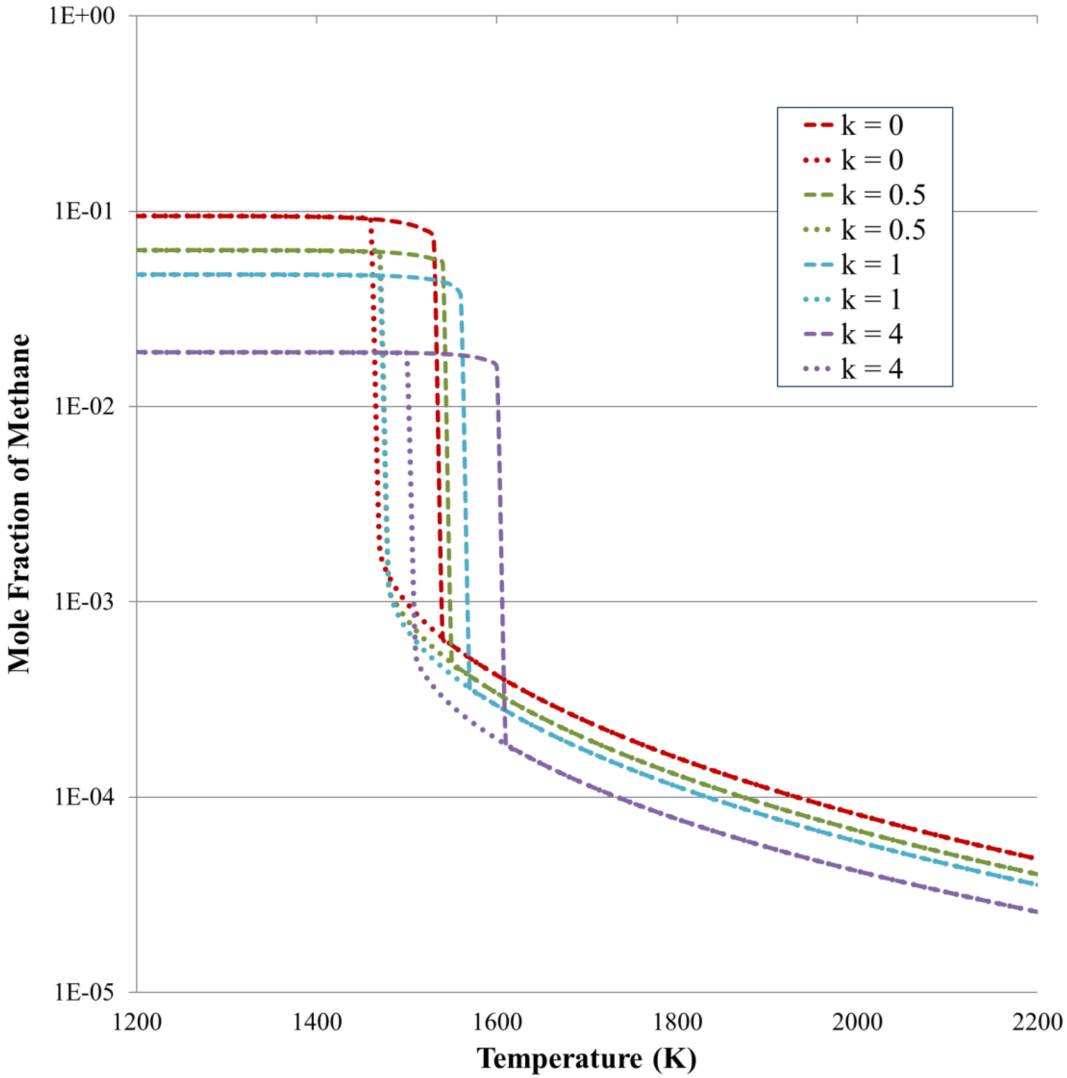
Air Inlet Temperature = 500 K;
Fuel Inlet Temperature = 500 K;
Recirculation Ratio, k = 1



Air Inlet Temperature = 500 K;
Fuel Inlet Temperature = 500 K;
Recirculation Ratio, k = 2



Results - Variation of Mole Fraction of Methane with Recirculation Ratio (Isothermal)



Conclusion

- The disappearance of ignition and extinction points and a monotonic steady-state temperature behavior of flameless-type of combustion process is shown for the first time using a detailed combustion mechanism.
- The transition to such a monotonic steady-state behavior seems to be primarily determined by the residence time (or volume for a constant mass flowrate system) of the reaction process.
- Recirculation, while necessary for the temperature rise needed for ignition as well as for low NOx emission, seems to delay the transition to flameless regime.
- Further studies on the practically accessible flameless conditions relevant to gas turbines for low NOx emission operation will be carried out.

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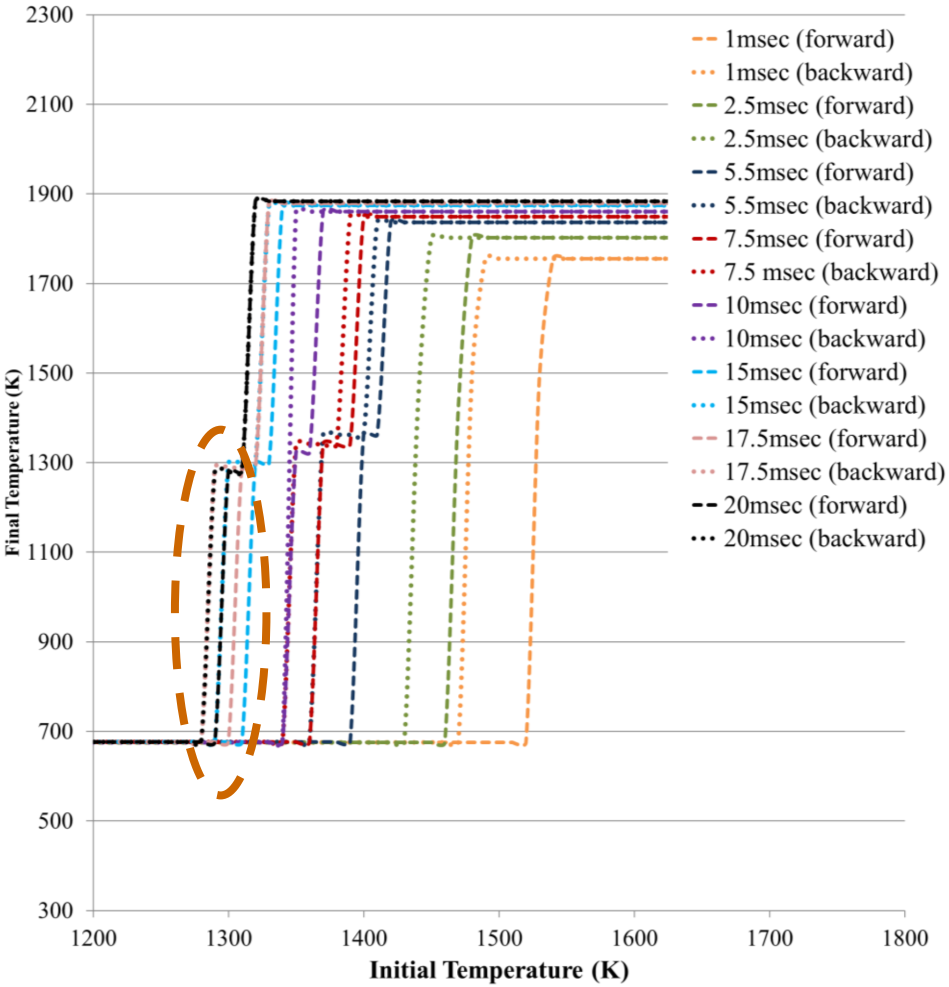
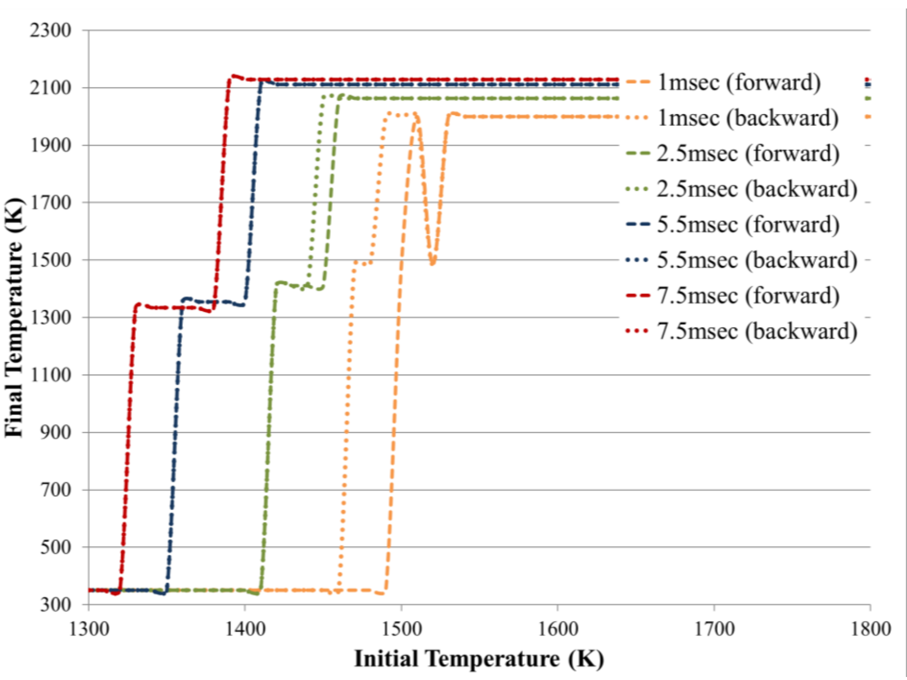
QUESTIONS

Results – Possible Low Temperature Activity



Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0.5 ; Recirculated Stream Temperature = 1250 K

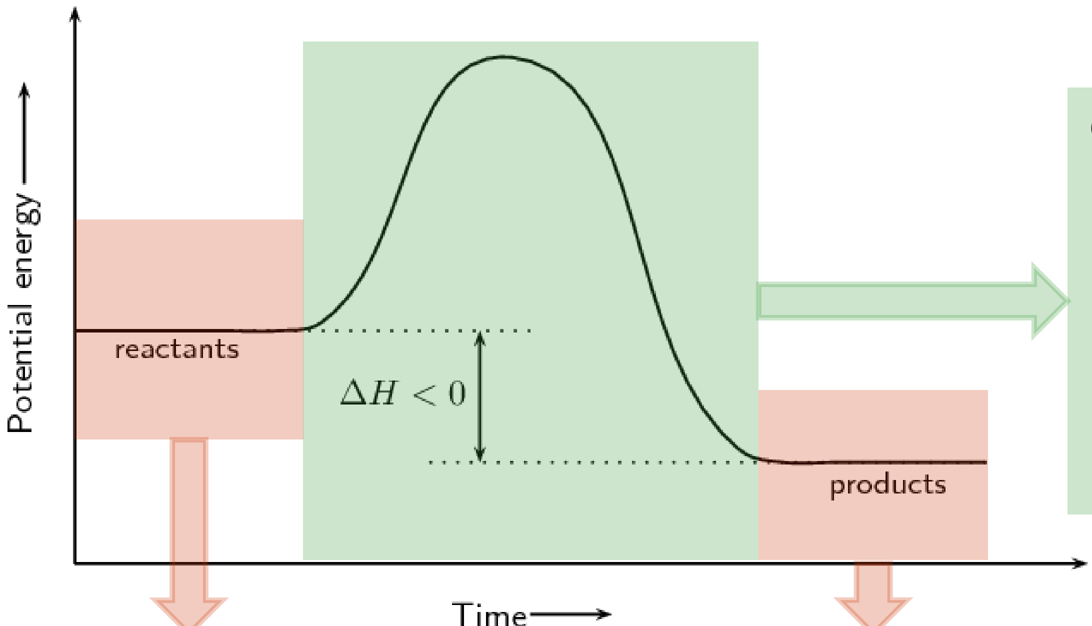


Air Inlet Temperature = 350 K; Fuel Inlet Temperature = 350 K; Recirculation ratio, k = 0

Literature Review - Combustion

Hydrocarbon + Oxidizer + Inert → Oxidized Reactant Molecules + Inerts

REACTANTS **PRODUCTS**



Complex Chemical Reactions
Depends on activation energies, kinetic rate laws, and other chemical properties.

State of Thermodynamic Equilibrium
Depends on temperature, pressure, molecular/atomic properties of reactant species.

HIGHLY COUPLED!

Literature Review – Chain Reactions

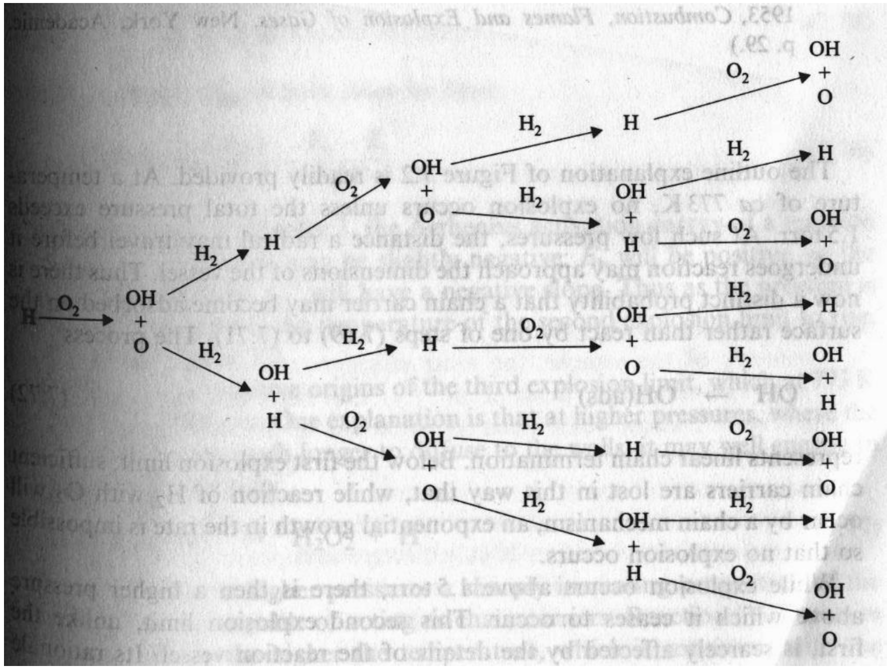
- Combustion is a complex chain chemical reaction in which active intermediate particles/species/centers react with reactants or other intermediate substances to form both combustion products and new active centers.
- **Chain Initiation:**

  Process of formation of active centers.
- **Chain Propagation:**

  Conservation of the active centers formed.
- **Chain Termination:**

  Loss of active centers.
- **Chain Branching**

  Proliferation of active centers.



Literature Review – Autoignition

- The main contributors to combustion heat release are the CO_2 and H_2O reactions.
- The concentration of active centers (n) available to form CO_2 and H_2O is crucial to the success or failure of the combustion process.
- The time variation of these active centers is given by,

$$\frac{dn}{dt} = W_o + (f - g)n$$

where, W_o – rate of creation of active centers

f / g – rate constants for chain branching / termination

$(f - g) < 0$ → NO COMBUSTION REACTION

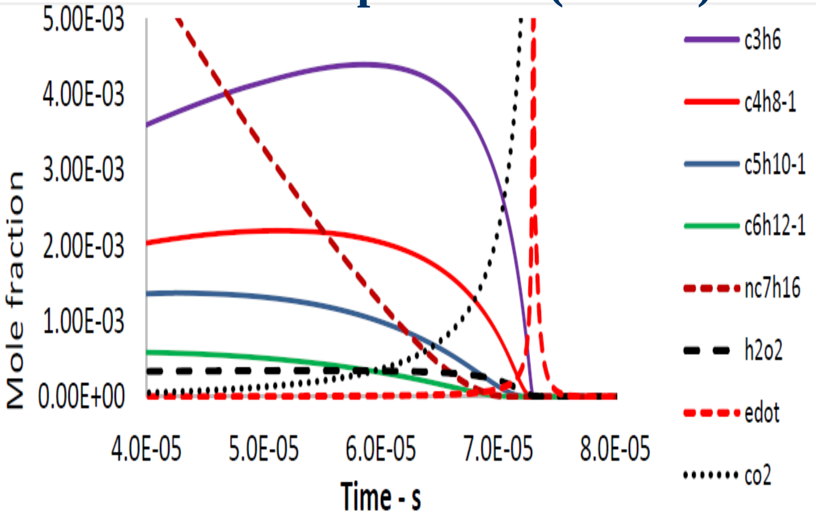
$(f - g) \geq 0$ → COMBUSTION REACTION

- Autoignition is the **critical temperature** at which (f – g) equals zero and the active centers produced are available to effect the heat release reactions for a specified reactor **residence time**.

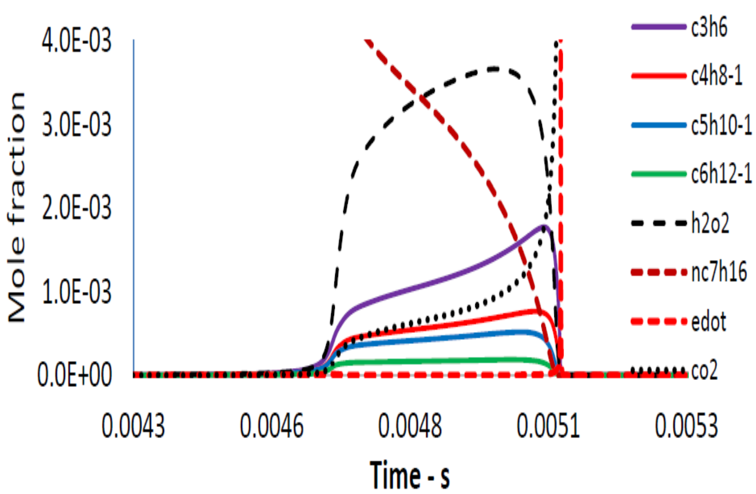
Literature Review – Autoignition of Hydrocarbons

Practically, autoignition can also be defined as the **critical time** at which (f – g) equals zero for a specified **reactor temperature**. No ignition is observed below this reactor residence time.

Initial Temperature (1300K)



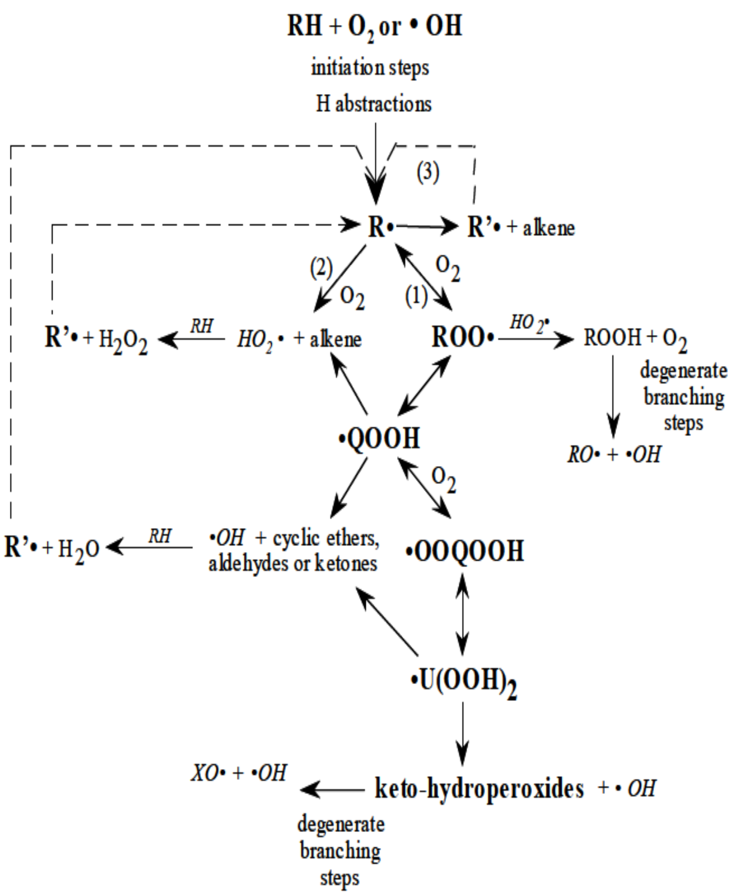
Initial Temperature (700K)



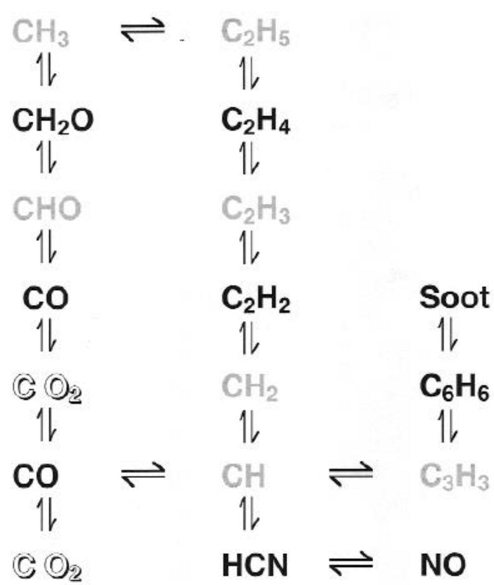
- OH active centers cannot grow explosively (above equilibrium) until fuel is fully consumed.
- (f – g) of OH species is kept negative by reaction with fuel species.

- OH active centers cannot grow explosively until temperature reaches the dissociation threshold of H_2O_2.
- (f – g) of OH species is kept negative by chain termination reaction to produce H_2O_2.

Low Temperature Reaction Process



CO_2/Soot Production



High Temperature Reaction Process