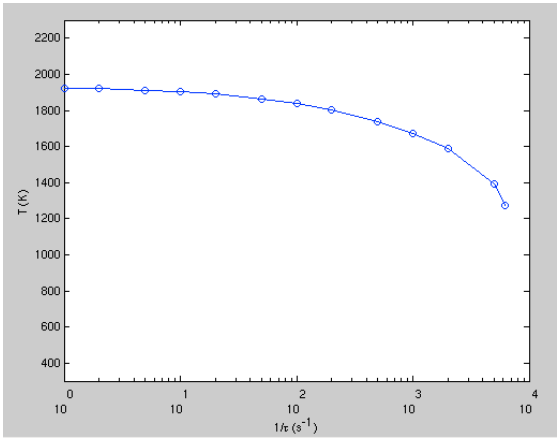
Chemical Engineering 641

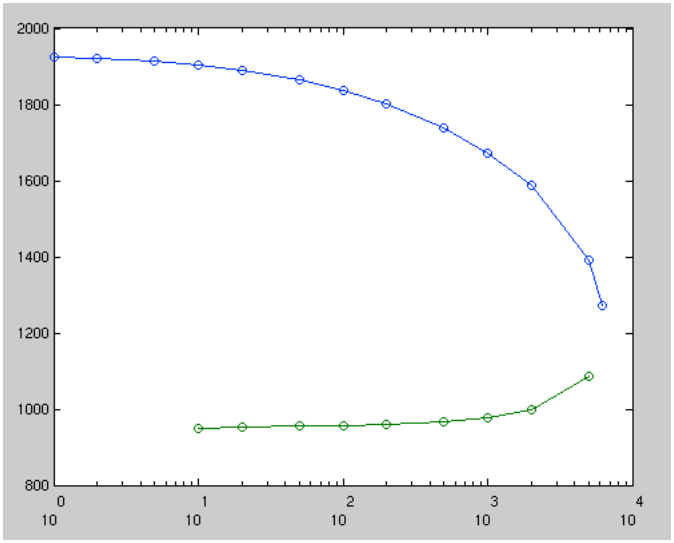
Combustion Modeling

Reactors

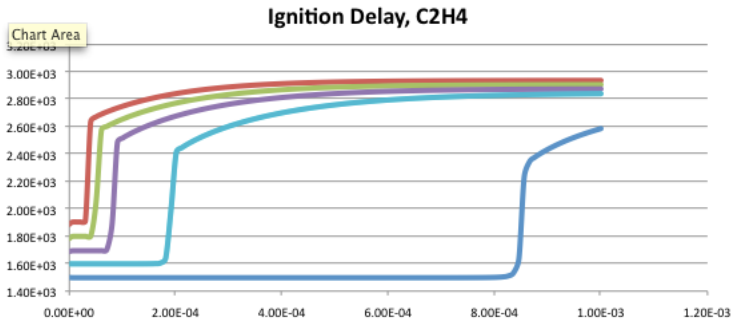
PSR



- Stoichiometric CO + 0.5H_2 flame with T_{in}=300 K



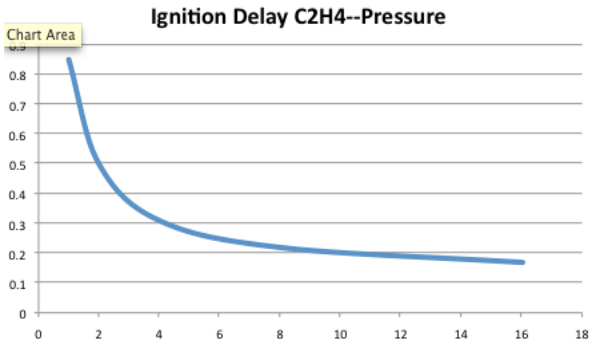
Ethylene Ignition Delay



- Best definition at max slope.
- Exponential increase in delay time with initial temperature.
- Adiabatic combustion in a PFR requires a high initial temperature

Ignition Delay, C2H4, Pressure

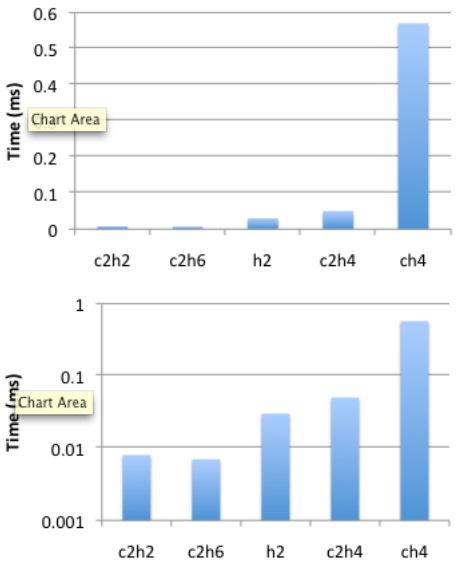
5



Delay time (ms), versus pressure (atm)

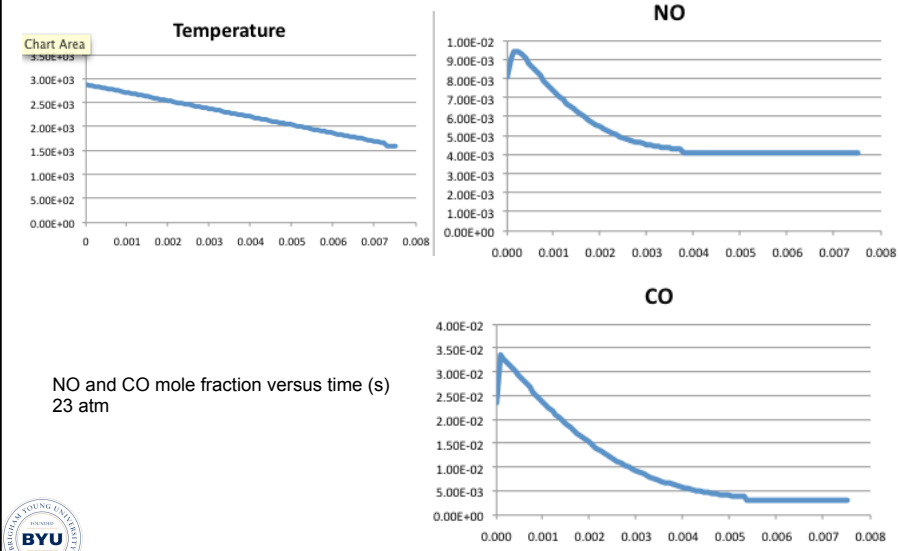
Ignition delay—fuels

6



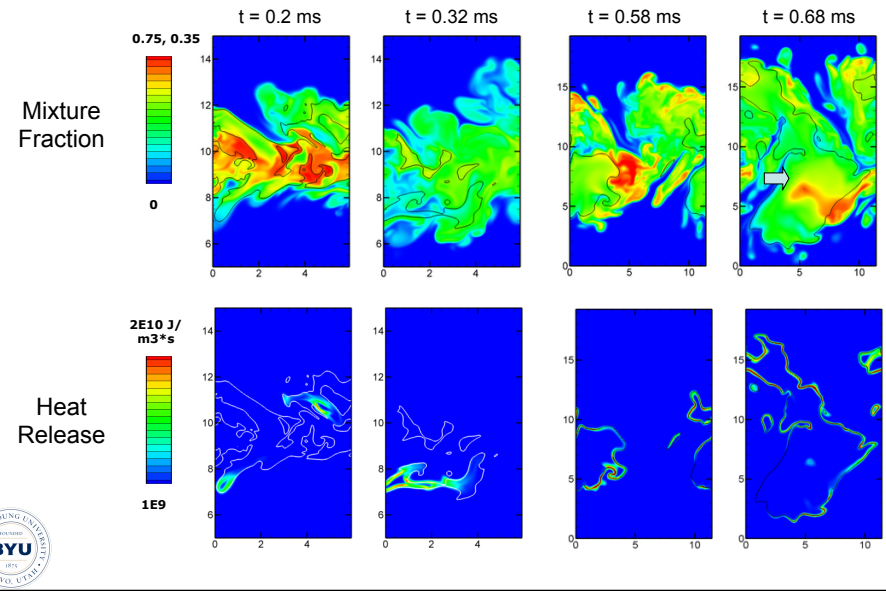
1800 K, 1 atm

Engine Expansion Stroke



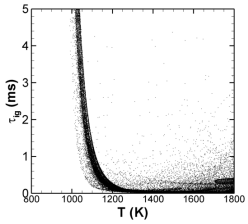
NO and CO mole fraction versus time (s)
23 atm

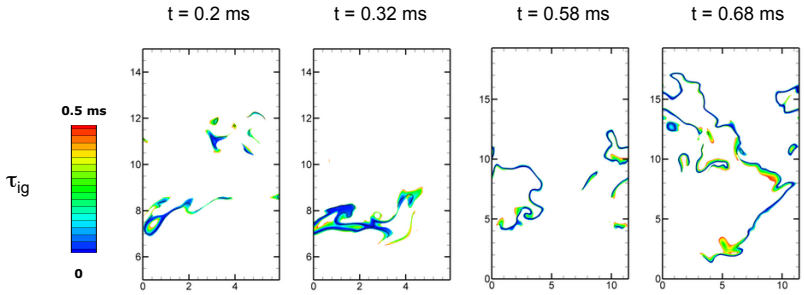
Mixture Fraction and Heat Release Evolution



Homogeneous Ignition Delay Time

- Ignition delay field of local DNS state computed pointwise using Senkin
- Crop values longer than 0.5 ms
- Possible ignition occurs in a partially burnt mixture
- Ignition delay fields are thin and confined to flame regions

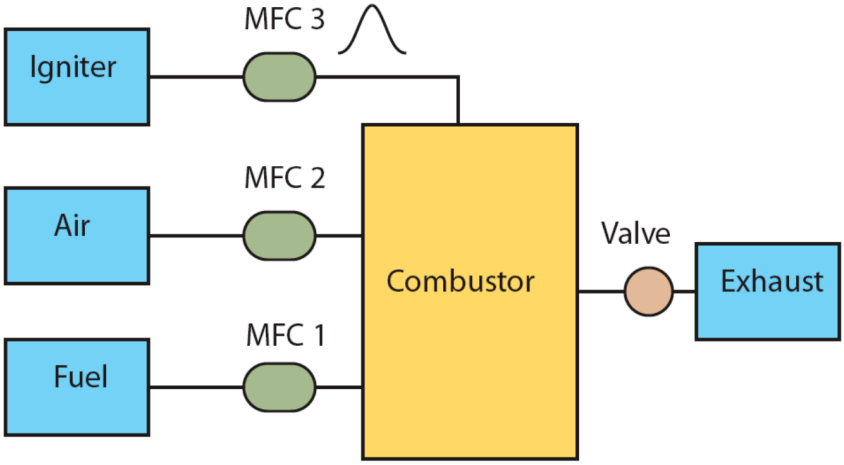




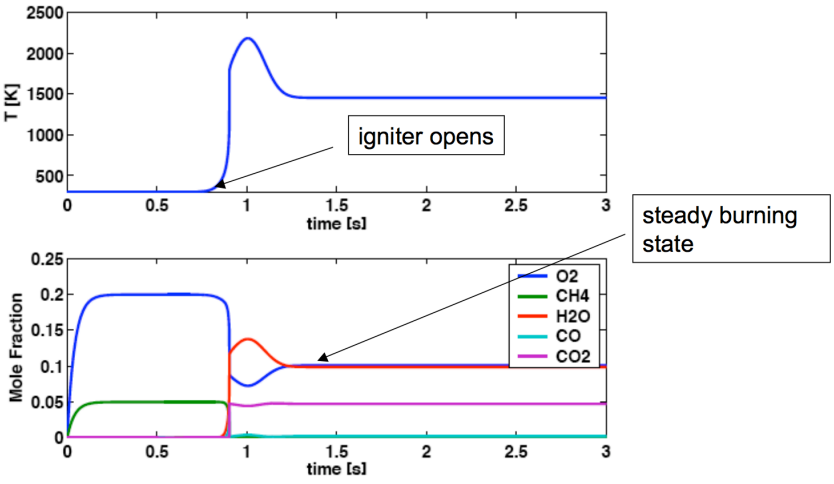
Engine NOx, CO

- Engine example
  - Model NOx and CO formation in an engine
  - Inlet = adiabatic (or not) equilibrium products at constant volume at TDC.
    - Better yet, use a reactor network of two batch reactors: one for the initial combustion, and one for the expansion stroke
  - Run a variable volume batch reactor with an engine stroke to watch pollutant changes.
  - Vary velocity RPM, heat loss, EGR
  - Compare Otto and Diesel

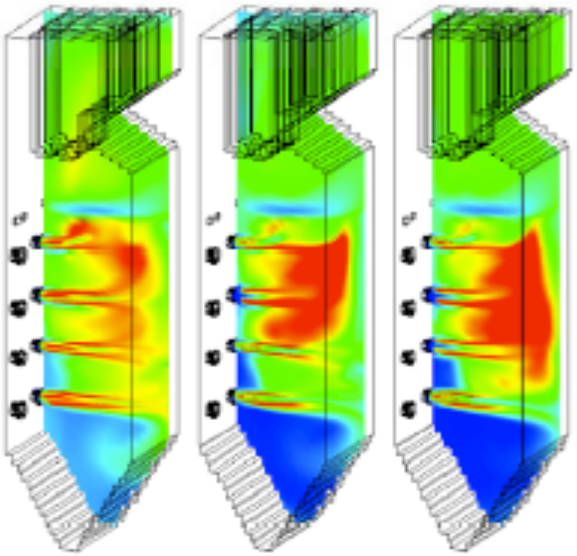
Combustor



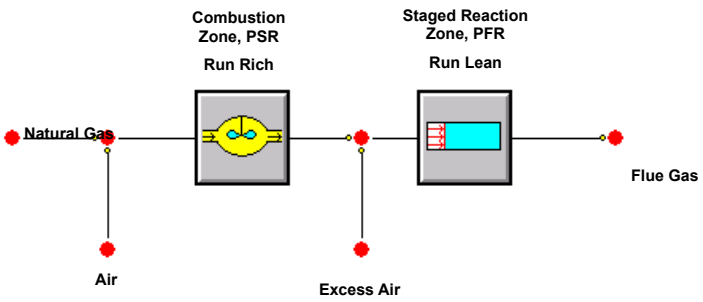
Combustor



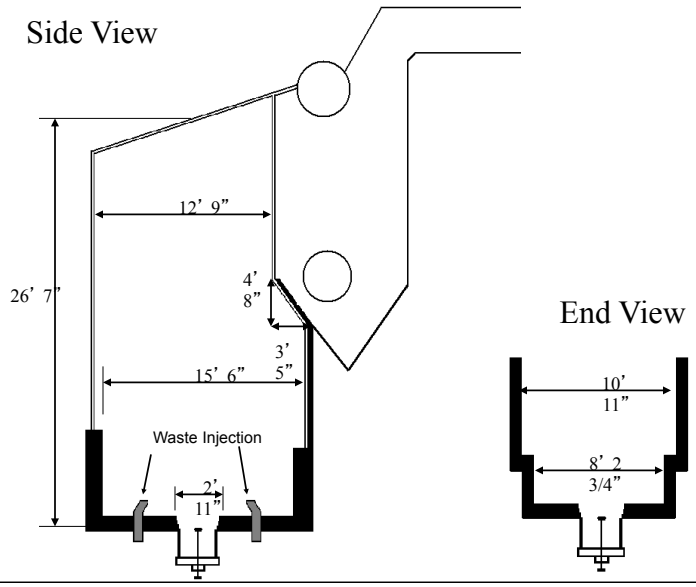
Combustor: OFA



Combustor: OFA



Reactor Netork: Boiler Schematic



Kinetic Model Description

- Model the flame zone with a perfectly stirred reactor (PSR) for a short time, operating at the adiabatic flame temperature. Model the oxidation zone with a plug flow reactor (PFR) for a long time. The PFR is run assuming several isothermal temperatures, and the time required for 99.99% destruction is found.
- The following operating conditions are assumed:
  - Firing rate: 129 MMBtu/h
  - Burner stoichiometric ratio: 1.3

Entrainment Model Diagram