

# Combustion

*I think I lost all the previous notes*

- Most combustion systems reach temperatures much higher than 1250K past which stable products are formed.
- Dissociation of the stable species occurs with a variety of radical reactions.
- The flame temperature here is the heat added to the system for the reaction if we consider it in some volume.
- It's the temperature that the products exist in.
- The enthalpy of combustion is heavily dependent on the stoichiometry of the products as this is that main difference in enthalpy formation of the products to the reactants.
- The formation of products is dependent on flame temperature and pressure (as in what dissociation reactions take place).
- Looking at the reaction rate, if we take the collision frequency as  $Z_{ab}$  with the fraction of molecules that have enough energy (changed by these collisions and/or changes in pressure) giving by the Boltzmann factor  $\exp(\frac{-E}{RT})$
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$$RR = Z_{ab} \exp(\frac{-E}{RT})$$

## Notes

*from lectures*

- What we have fundamentally is a fuel and some oxidizer (like air or O<sub>2</sub>).
- If we can generate enough energy to dissociate the chemical energy held within the bonds of the fuel we create heat through the energy differential of the reactants (fuel and air) and its products (H<sub>2</sub>O and CO<sub>2</sub>).
- The change in energy is huge (like 2000K). This huge gradient leads to the formation of pollutants.
- Why Hydrocarbons?
  - Very high energy density.
  - Chemically stable at ambient temperatures.
- A good point is that something like a gas turbine, or scramjet (military uses) are some of the most engineered things in the world.
- In theory, a perfect combustion reaction should result in carbon dioxide and water, imperfections in this process result in particulates.
- Walking the soot, Nox line is hard (why?).
- As the flame temperature increases, so do the oxides of nitrogen. The flame temperature is a function of the equivalence ratio. It determines the reaction rate throughout the combustion process. Lecture 5 green area.
- The *stoichiometric mixture fraction* is the minimum quantity of air we need to convert a quantity of fuel to its reaction products (carbon dioxide and water).

- In the fuel rich case, we haven't given the fuel enough air to make all its products. The intermediates it generates are undetermined.
- Lean reaction will distribute energy from fuel a bit more amongst the oxidizer molecules if not done perfectly.
- 21/11/22 11:06:48
  - Looking at performance as well as safety, for instance, lead improved performance but lead had to start being taken out.
  - Ethyl groups added to lead to make it soluble in gasoline. Tetra ethyl lead.
  - RON (Research octane number) is how slow the chain reaction is.
    - \* Looked at otto cycle. On volume reduction, the pressure increases, but so does the temperature which may fuel radical reactions that can keep heat in the system.
    - \* Usually bottom dead center and top center ratio 16:1.
    - \* Using this engine, what's the ignition time (RON)
  - Benzene is carcinogenic whereas other legal standards looking at octane number.
  - Cetane no. is the opposite of the octane number.
  - Gas chromatography graph shows the size of molecules in fuel composition. The shorter the time the smaller the molecules (they get filtered quicker).
  - Viscosity of fuel is important as you look at evaporation that needs to happen on short timescales in the Otto cycle.
  - Crank angle degree, the height of the piston.
  - The high temperature reactivity is similar despite the fuel because of the beta bond (?).
  - combustion assignment 2
- 23/11/22 11:03:59
  - H2H4 (ethylene), breaking of beta bond scission. The reaction is endothermic.
  - Alpha, beta, position relative to radical site.
  - In the methane system, there's no beta system problem. If the beta bond breaks you just go back to reactants.
  - Look for propane (C3H6), Formaldehyde (CH2O) in computations.
  - $C_xH_y + O \rightleftharpoons CO_2 + H_2O$  where the arrows are a universe of intermediates that increase and decrease temperature until a large exothermic reaction starts to finally get to the products. The left is technically time at zero and the right time at equilibrium but the in between is complicated.
  - Oxides generally lower in free energy than hydrocarbon (formation exothermic).
  - Incremental release of chemical enthalpy of the fuel.
  - Lead used to stop knock (the autoignition in the unburned gas).
  - Rocket system that doesn't shake itself apart (combustion instability) thermo acoustic interaction, Von Braun.
  - At higher distances from the injector tip, the equivalence ratio is

- lower. It's a gradient in the chamber.
- Hydrocarbons: Alkanes and aromatics. C-C bond rather than 4 Hydrogen bonds, aromatic (hexagonal shape). Resonance structure, the radical is propagated in a ring.
    - \* Aromatics are a precursor to soot.
  - Very complicated chain mechanism for how a single radical might be generated. Something called 'Q' was introduced. End up with a 'keto-hydroperoxide'. Temp lower than 950K you will end up with water because of the OH radical. It's the process of oxidation of food.
  - $\text{fuel} + \text{O}_2 \rightarrow \cdot R + 2 \cdot \text{OH} + \text{RH}$
  - H2O2 decomposes to make two OH which make water by hydrogen abstraction (temperature increase).