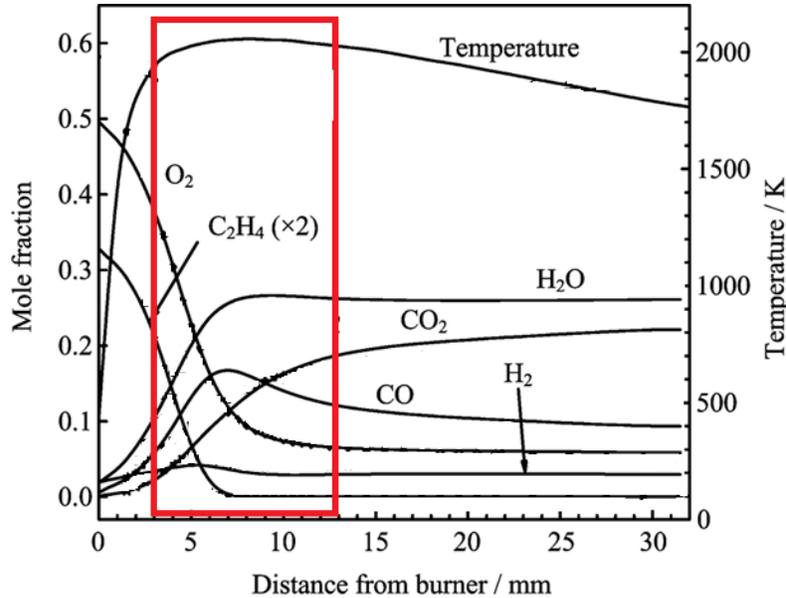
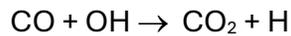
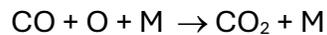
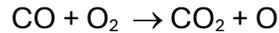


ME 501 S25 Homework #3 Due 2/18/25

- 1) In most hydrocarbon combustion scenarios, carbon in the fuel is first oxidized to CO, and then the CO is further oxidized to CO₂. See, for example, this depiction of a premixed flame where reactants enter on the left and proceed to products on the right.



In the region in red, CO is converted to CO₂, and CO₂ concentration rises accordingly. Consider now three possible reactions that could contribute to this conversion:



Let's examine how much each contributes to the conversion by first examining their efficiency.

- For each of the three reactions, find data at 2000 K and list the rate parameters (A, n, E_a) that you think would best model the reaction. Justify your choice.
- Calculate the fraction of collisions for each reaction that would lead to reaction at 2000 K and 1 atm total pressure. For the reaction with O, compare reaction rate to collision rate of CO and O.
- Given the relative concentrations in the problem as shown in the figure above, and assuming O and OH are of mole fractions of order $1e-2$ to $1e-3$, which of the three reaction paths do you think is the path that leads to the most CO conversion. Why?

- 2) Consider the recombination reaction $O + O + M \rightarrow O_2 + M$. From our fundamental form of chemical kinetics, we can say that:

$$\frac{dN_O}{dt} = -2kV[O]^2[M]$$

Which is simplified to the more common form, in the case of constant volume, as:

$$\frac{d[O]}{dt} = -2k[O]^2[M]$$

However, in the case that volume is not constant, the top equation holds, but the bottom does not.

Consider a system where:

- i) The only element is O, and the only species are O and O₂
- ii) Only the recombination reaction is occurring (no dissociation)
- iii) You start with a mole fraction of 0.1 of O
- iv) Temperature and pressure are held constant (1 atm, 300 K)
- v) The reaction rate for recombination is $1e-32 \text{ cm}^6/\text{molecule}^2 \text{ s}$ (3rd order)

Starting with the top equation, and noting that $X_O = N_O/N$, that $N = N_O + N_{O_2}$, and that $[M] = N/V = P/R_u T$, derive an expression for dX_O/dt as a function of X_O and constants.

Integrate this expression (you can use a solver, but you should get a fairly simple analytic solution).

Using your expression, calculate the time for the system to react from the initial state until an atomic O mole fraction of 0.001 is reached.