(GEE 430/HE 430) Elementary rxns

**Rxn 'mechanisms': chain rxns!**

- In combustion, as well as other chem rxns, it is important to distinguish between (overall) rxn stoich and elementary steps (collision events) of the reacting molecules (or species).

  - e.g., \( \text{H}_2 + 0.5 \text{O}_2 = \text{H}_2\text{O} \) is NOT an elementary rxn.

  - Initiation step(s)
    - e.g., \( \text{CH}_4 \rightarrow \text{CH}_3 + \text{H} \) production of radicals
    - \( \text{H} \cdot \text{C} \cdot \text{H} \cdot \text{H} \cdot \) homolytic scission of the C-H Bond

  - Propagation steps
    - \( \text{H} \cdot + \text{O}_2 \rightarrow \text{OH} + \cdot \text{O} \)
    - \( \text{CH}_3 + \text{CH}_4 \rightarrow \text{C}_2\text{H}_6 + \cdot \text{H} \)
    - \( \cdot \text{H} + \text{CH}_4 \rightarrow \cdot \text{H}_2 + \text{CH}_3 \cdot \)
    - etc.

  - Termination step(s)
    - \( \cdot \text{H} + \cdot \text{H} \rightarrow \text{H}_2 \)
    - \( \text{CH}_3 + \cdot \text{H} \rightarrow \text{CH}_4 \cdot \)
    - etc.

- Similar to nuclear fission (\( 3...9...27...\) explosions?)

- **Complex!**
  - Powerful tool for solving many simult. eqns: CHEMKIN
  - Both kinetics and thermodynamics + transport (mixing)

- See CRI-Mech web site!!

- Example of a reversible rxn

- Reaction stoichiometry essentially balanced