Planar Detonations and Detonation Structure

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Methane Flame

ZND Model: Detonation Structure

• Generally, molecular collisions that equilibrate $p$ and translational energy precede chemical reactions
  – characteristic momentum transfer collision < 1 ns
  – characteristic chemical reactions > O(1 µs)

• Suggests detonation is leading shock followed by reaction zone
  – shock raises $p$ and $T$
  – $M$ goes subsonic
  – autoignition after delay
  – heat release, $T \uparrow$, $p \downarrow$ like deflagration

Zeldovich, von Neumann, Döring
Weak Detonations

- After leading shock wave, flow reduced to subsonic

- To achieve weak detonation, flow must reaccelerate to $M_2 > 1$

- If induction/reaction zones only have heat release
  - would violate 2nd Law
    - can’t go from subsonic to supersonic 1D flow with heat addition ($q > 0$ always drives toward $M = 1$)

- Look at path on Rayleigh Hugoniot

  - To go from d to e, need negative heat release (endothermic reactions)
    - requires chemistry to “overshoot” equilibrium
Chapman-Jouget Detonations

- No weak (unallowed), strong (unstable) detonation
- Only leaves Chapman-Jouget solution
  - C-J detonation is planar detonation solution
- We have constraint to add to 5 conservation and state equations: $M_2=1 \Rightarrow 6$ eqs., 6 unknowns!

CJ Detonation Equations

- Find detonation wave speed, $D \equiv u_1$
  and product properties ($\rho_2/\rho_1$, $p_2/p_1$, $T_2/T_1$, $u_2$)
- CJ constraint
  $$u_2 = a_2$$
- Mass
  $$D = \frac{\rho_2}{\rho_1} u_2 = \frac{\rho_2}{\rho_1} \sqrt{\gamma_2 \frac{R}{W_2} T_2}$$
- Rayleigh
  $$\gamma_2 M_2^2 = \frac{1 - p_1/p_2}{\rho_2/\rho_1 - 1} \quad \frac{\rho_2}{\rho_1} = 1 + \frac{1}{\gamma_2} \left( 1 - \frac{p_1}{p_2} \right)$$
  For strong detonation, $p_2/p_1 \gg 1$
  $$D = \frac{\gamma_2 + 1}{\gamma_2} \sqrt{\gamma_2 T_2 R/W_2} = D(\gamma_2, W_2, T_1)$$
CJ Detonation Equations

- Virial, P.G. 
  \[ \frac{p_2}{p_1} = \frac{T_2 / \overline{W}_2}{T_1 / \overline{W}_1} \]

- In above equations, still need product composition to get \( \gamma_2 \), \( W_2 \) and \( T_2 \)
  - high \( p, T \) \( \Rightarrow \) assume products in chem. equilibrium
  - small changes in radical populations/pollutants will not change product properties significantly

- Hugoniot 
  \[ h_2 - h_1 = \frac{1}{2} (p_2 - p_1) \left( \frac{1}{\rho_1} + \frac{1}{\rho_2} \right) \]
  \[ e_2 - e_1 = \frac{1}{2} (p_2 - p_1) \left( \frac{1}{\gamma_2 \rho_2} \right) \approx \frac{R T_2}{2 \gamma_2 \overline{W}_2} \]

  a sol’n method: guess \( p_2, T_2 \); find \( Y_i \Rightarrow \rho_2, \rho_1 \Rightarrow D, p_2, p_1 \Rightarrow T_2 \); Iterate

Example: \( H_2 \)-Air CJ Detonation

- 298 K, 1 atm

![Graph showing velocity vs. hydrogen percentage]
Detonation Limits

- 298 K, 1 atm
- Don’t get steady, self-sustained detonation if mixture is too rich or too lean
- Not equil. issue – kinetics, losses

3D Detonation Structure

- 1-d detonation
- 2-d/3-d detonation

from Timmes et al., Astrophysical J., 938-954 (2000)
Front Propagation

from Timmes et al., Astrophysical J., 938-954 (2000)

Experimental Evidence

- Smoke foil records triple point tracks

24 mm

34 mm
Triple Point Region

from Numerical Simulations of Gaseous Detonations, www.cacr.caltech.edu

AE/ME 6766 Combustion