Detonation Situations

- Here are some example situations where detonation waves occur
  - underground (coal) mine explosions
  - pipeline explosions
  - propulsion
    - pulsed detonation engines (PDEs)
    - rotating detonation engines (RDEs)
  - stellar detonations

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Overview

- Goal of this section are:
  1. examine the likely structure of a 1-d (planar) detonation wave and explain the absence of weak planar detonations
  2. outline the solution process for and behavior of planar Chapman-Jouguet (CJ) detonations
  3. introduce the 3-d nature of quasi-planar detonation

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 $> \mathcal{O}(1 \mu s)$

- Suggests detonation is leading shock followed by reaction zone
  - shock raises $p$ and $T$
  - $M$ goes subsonic
  - induction delay/autoignition
  - heat release, $T \uparrow, p \downarrow$ like deflagration
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 2\textsuperscript{nd} Law
  - can’t go from subsonic to supersonic 1D flow with heat addition ($q > 0$ always drives toward $M = 1$)

Weak Detonations

- Look at path on Rayleigh Hugoniot
  - To go from d to e, need negative heat release (endothermic reactions)
    - requires chemistry to “overshoot” equilibrium
Chapman-Jouguet Detonations

- No weak (unallowed), strong (unstable) detonation
- Only leaves Chapman-Jouguet 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

- Goal: find CJ detonation wave speed, \( u_1 \equiv D_{CJ} \) and product properties \((\rho_2/\rho_1, p_2/p_1, T_2/T_1, u_2)\)
- CJ constraint
  \[ u_2 = a_2 \]  
  \[ u_1 = \frac{\rho_2}{\rho_1} u_2 \]  
  \[ D_{CJ} = \frac{\rho_2}{\rho_1} a_2 \]  
- Mass
  \[ u_1 = \frac{\rho_2}{\rho_1} \]  
  \[ \frac{a_2^2}{p_2/\rho_2} \]  
  \[ D_{CJ} = \frac{\rho_2}{\rho_1} a_2 \]  
- Rayleigh
  \[ \frac{a_2^2}{p_2/\rho_2} = \frac{1 - p_2/p_1}{\rho_2/\rho_1 - 1} \]  
  \[ \frac{a_2^2}{p_2/\rho_2} = \frac{1 - p_2/p_1}{\rho_2/\rho_1 - 1} \]  
- Hugoniot
  \[ h_2(T_2,Y_2) - h_1 = \frac{1}{2} (p_2 - p_1) \left( \frac{1}{\rho_1} + \frac{1}{\rho_2} \right) \]  
  \[ h_2(T_2,Y_2) - h_1 = \frac{1}{2} (p_2 - p_1) \left( \frac{1}{\rho_1} + \frac{1}{\rho_2} \right) \]
CJ Detonation Eq’ns.: Ideal Gas

- Need state eqn’s
  \[ p_2 = \frac{\rho_2}{\rho_1} \frac{T_2}{T_1} \]
  \[ a = \frac{\gamma R}{W} T = \sqrt{\frac{p}{\rho}} \]
  \[ D_CJ = \frac{\rho_2}{\rho_1} \sqrt{\gamma_2 \frac{R}{W_2} T_2} \]

- For ideal gas
  \[ h_2 = h_2(T_2, p_2, Y_{i2}) \]
  \[ \gamma_2 = \gamma_2(T_2, Y_{i2}) \]
  \[ W_2 = W_2(Y_{i2}) \]

- Products assume chem. equil. \( Y_{i2} = Y_{i2}(T_2, p_2) \)

- For high \( M, p_2/p_1 \gg 1 \)

  \[ \rho_2/\rho_1 = (\gamma_2 + 1)/\gamma_2 \]
  \[ D_CJ \approx \frac{\gamma_2 + 1}{\gamma_2} \sqrt{\gamma_2 \frac{R}{W_2} T_2} \]

- Small changes in minor species do not change product properties significantly

CJ Detonation Solution Method

- Need to solve these equations (including chemical equilibrium) simultaneously
  - available in various equil. solvers (e.g., GasEq, CEA)
- By “hand” can use simple procedure for \( p_2/p_1 \gg 1 \)
  1) guess \( T_2, W_2, \gamma_2 \)
  2) get \( p_2 \) from (VI.3)
  3) solve chem. equil. at \( (T_2, p_2) \) to find \( e_2, \gamma_2, W_2 \)
  4) compare \( e_2, T_2 \) with version of (V.10)
  5) iterate until requirement met, then \( D_CJ \approx \frac{\gamma_2 + 1}{\gamma_2} \sqrt{\gamma_2 \frac{R}{W_2} T_2} \)
Example: H₂-Air CJ Detonation

- 298 K, 1 atm
- Solution of full set of eqns. with chemical equilibrium solver

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)

AE/ME 6766 Combustion

Triple Point Region

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

AE/ME 6766 Combustion
Front Propagation

Experimental Evidence

- Smoke foil records triple point tracks

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