Numerical Simulation of Hydrogen Detonations and Application in Enclosed Environments

Luc Bauwens

University of Calgary, Mechanical & Mfg Engineering

First European Summer School on Hydrogen Safety

Belfast, August 2006
Thanks

- To Vladimir Molkov for the invitation
- To Elaine Oran for her considerable help (movies, pictures, papers, advice)
- To Koichi Hayashi & N. Tsuboi for their pictures
Overview

- Motivation
- Requirements for simulation of high speed flow (review)
- Chemical reaction
- Hydrogen: chain-branching
- Two examples
  - Hydrolyser
  - Tunnel
Motivation

- Hydrogen: detonates over wide range of concentrations
- Detonations: quite violent and destructive
- Ignition: still unpredictable
- Enclosed environment may be problematic
Gas dynamics

- Perhaps better mathematical background than for low speed flow?
- Looks easy: just unroll time-derivatives?
- Real issue: dealing with shocks and expansion waves
  - Conservation
  - Flux limiting
  - Entropy condition
Conservation

- Conservation laws
  - Example: 1-D mass: for arbitrary $x_l$ and $x_r$,

\[
\frac{d}{dt} \int_{x_l}^{x_r} \rho dx + \rho u|_{x_l} - \rho u|_{x_r} = 0
\]
Conservation paradox

- Expanding etc., recover usual continuity
- Remember, for inviscid non-conducting conservation (mass, momentum, energy) -> isentropic
- However, from the Rankine-Hugoniot equations (continuity of fluxes across shock), a shock is NOT isentropic.
Burger's equation

- Similar (simpler) problem:
  \[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \]

- Solved on characteristics:
  \[ \frac{dx}{dt} = u(x, t), \quad u(x, t) = u(x_0, 0) \]

since

\[ du = \frac{\partial u}{\partial t} dt + \frac{\partial u}{\partial x} dx = 0 \]
Burger's Equation

- Consider IC at $t = 0$:
- Solution:

\[ u = 1 \]
\[ u = 0 \]
\[ u = ? \]
Burger's Equation

- What happened? Multiple solutions?
- What if the equation actually were the conservation law:

\[
\frac{d}{dt} \int_{x_l}^{x_r} u dx + \frac{u^2}{2} \bigg|_{x_r}^{x_l} - \frac{u^2}{2} \bigg|_{x_l} = 0
\]

- Then we can construct a shock solution: \( x < x_s \): \( u = u_l \) but \( x > x_s \), \( u = u_r \)
- Replacing, we find \( x_s = \frac{u_l + u_r}{2} = 1/2 \)
But note that Burger's equation is consistent not only with the conservation above, but more generally with:

\[
\frac{d}{dt} \int_{x_l}^{x_r} u^n dx + \frac{nu^2}{n+1} \bigg|_{x_r} - \frac{nu^2}{n+1} \bigg|_{x_l} = 0
\]

So,

\[
x_s = \frac{n}{n+1} \frac{u_l^{n+1} - u_r^{n+1}}{u^n_l - u^n_r}
\]
Burger's Eqn: summarizing

- Differential equation could have come from infinitely many conservation laws
- Shock speed depends upon the specific conservation law
- So shock speed not determined by the differential equation
Conservative schemes

- Exact discrete conservation (on the grid)
- Arbitrary schemes: error depends upon mesh size both
  - Directly
  - Through the jump in the function in neighboring grid points
- If conservative: only the former. So, error becomes small with mesh even if jump
Flux Limiting

- Issue is oscillations close to shocks
- Avoiding oscillations: monotone schemes
- Godunov theorem: linear conservative monotone schemes at most first order accurate
- First order: quite poor, not good enough
Flux Limiting

- Oscillations arise because fluxes oscillate from one time step to next
- Crucial idea: limit fluxes where they oscillate
  - Near shocks, accuracy deteriorates to 1\textsuperscript{st} order
  - Elsewhere, higher order
- Proposed independently by Jay Boris and Bram van Leer in the early seventies
- Nonlinear schemes
Entropy condition

- Burger's eqn, with IC:
- Solution:
Entropy condition

- What if IC ($\Omega$ small):
- Shock: “invent information”
- Solution: fan
Gas Dynamics-Summary

- Pretty good
- But near shocks: first order at best
- Handles shocks and expansions transparently
- Explicit: CFL (Courant-Friedrichs-Lewy) condition for stability
- However even implicit: near-CFL for accuracy
- Various schemes: TVD, Godunov, ENO, FCT...
Chemical Kinetics

- Two key issues:
  - How good is the model?
  - Stiffness

- How good?
  - Hydrogen air is the simplest and best known
  - However, typically not calibrated against detonations
  - Uncertain at high pressures
## Chemical Kinetics (example)

<table>
<thead>
<tr>
<th>$j$</th>
<th>Reaction</th>
<th>$A_j$</th>
<th>$\beta_j$</th>
<th>$E_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{OH} + \text{OH}$</td>
<td>$1.70 \times 10^{13}$</td>
<td>0.00</td>
<td>47,780</td>
</tr>
<tr>
<td>2</td>
<td>$\text{OH} + \text{H}_2 \rightleftharpoons \text{H}_2\text{O} + \text{H}$</td>
<td>$1.17 \times 10^{9}$</td>
<td>1.30</td>
<td>3,626</td>
</tr>
<tr>
<td>3</td>
<td>$\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$</td>
<td>$5.13 \times 10^{16}$</td>
<td>-0.82</td>
<td>16,507</td>
</tr>
<tr>
<td>4</td>
<td>$\text{O} + \text{H}_2 \rightleftharpoons \text{OH} + \text{H}$</td>
<td>$1.80 \times 10^{10}$</td>
<td>1.00</td>
<td>8,826</td>
</tr>
<tr>
<td>5</td>
<td>$\text{H} + \text{O}_2 + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$</td>
<td>$2.10 \times 10^{18}$</td>
<td>-1.00</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>$\text{H} + \text{O}_2 + \text{O}_2 \rightleftharpoons \text{HO}_2 + \text{O}_2$</td>
<td>$6.70 \times 10^{19}$</td>
<td>-1.42</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>$\text{H} + \text{O}_2 + \text{N}_2 \rightleftharpoons \text{HO}_2 + \text{N}_2$</td>
<td>$6.70 \times 10^{19}$</td>
<td>-1.42</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>$\text{OH} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$</td>
<td>$5.00 \times 10^{13}$</td>
<td>0.00</td>
<td>1,000</td>
</tr>
<tr>
<td>9</td>
<td>$\text{H} + \text{HO}_2 \rightleftharpoons \text{OH} + \text{OH}$</td>
<td>$2.50 \times 10^{14}$</td>
<td>0.00</td>
<td>1,900</td>
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<tr>
<td>10</td>
<td>$\text{O} + \text{HO}_2 \rightleftharpoons \text{O}_2 + \text{OH}$</td>
<td>$4.80 \times 10^{13}$</td>
<td>0.00</td>
<td>1,000</td>
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<tr>
<td>11</td>
<td>$\text{OH} + \text{OH} \rightleftharpoons \text{O} + \text{H}_2\text{O}$</td>
<td>$6.00 \times 10^{8}$</td>
<td>1.30</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>$\text{H}_2 + \text{M} \rightleftharpoons \text{H} + \text{H} + \text{M}$</td>
<td>$2.23 \times 10^{12}$</td>
<td>0.50</td>
<td>92,600</td>
</tr>
<tr>
<td>13</td>
<td>$\text{O}_2 + \text{M} \rightleftharpoons \text{O} + \text{O} + \text{M}$</td>
<td>$1.85 \times 10^{11}$</td>
<td>0.50</td>
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<tr>
<td>14</td>
<td>$\text{H} + \text{OH} + \text{M} \rightleftharpoons \text{H}_2\text{O} + \text{M}$</td>
<td>$7.50 \times 10^{23}$</td>
<td>-2.60</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$</td>
<td>$2.50 \times 10^{13}$</td>
<td>0.00</td>
<td>700</td>
</tr>
<tr>
<td>16</td>
<td>$\text{HO}_2 + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$</td>
<td>$2.00 \times 10^{12}$</td>
<td>0.00</td>
<td>0</td>
</tr>
<tr>
<td>17</td>
<td>$\text{H}_2\text{O}_2 + \text{M} \rightleftharpoons \text{OH} + \text{OH} + \text{M}$</td>
<td>$1.30 \times 10^{17}$</td>
<td>0.00</td>
<td>45,500</td>
</tr>
<tr>
<td>18</td>
<td>$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{HO}_2 + \text{H}_2$</td>
<td>$1.60 \times 10^{12}$</td>
<td>0.00</td>
<td>3,800</td>
</tr>
<tr>
<td>19</td>
<td>$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$</td>
<td>$1.00 \times 10^{13}$</td>
<td>0.00</td>
<td>1,800</td>
</tr>
</tbody>
</table>

*Extracted from Ref. 34 and used in Refs. 9 and 10.

Kinetic schemes

- Various levels of simplification
  - “Full” kinetics (some more “ful” than others)
  - Various levels of reduced schemes
  - Single (or two, or three) steps
- Even for oxygen-air (simplest)
  - Different schemes -> different results
  - None really matches cell size
  - (Typically calibrated for flames)
Stiffness

- Kinetics: very slow and very fast rates
  - (many orders of magnitude)

- “Regular” integration
  - Either unreasonably (impossibly) small step
  - Or step too big for fast rates -> instability

- “Stiff solvers” avoid instability

- No miracle: fast steps are NOT resolved
  - (= inadvertent scheme reduction...)


Chain-Branching

- Typical of hydrogen-oxygen

(From Dainton, 1965)
Simple Chain-Branching

- **Four-step model** (three-step: Short 1997)

  **Initiation**
  \[ R \xrightarrow{K_I} X \]  
  \[ r_I = f(T) \]

  **Branching**
  \[ R + X \xrightarrow{K_B} 2X + Pr \]  
  \[ r_B = f(T) \]

  \[ X \xrightarrow{K_w} Pr \]  
  \[ r_W = f(1/p) \]

  **Termination**
  \[ X + M + M \xrightarrow{K_G} Pr + 2M \]  
  \[ r_G = f(p^2) \]

  - Competition for specie X
  - Production/consumption \( a = (r_I + r_B)/(r_W + r_G) \)
  - \( A > 1 \): “explosion”
Simple Chain-Branching

Four step

Dainton 1965, $\text{H}_2+\text{O}_2$
Four Step: ZND Profiles

- **Induction zone**
- **Chain explosion zone**
- **Recombination zone**

**Mass Fraction**

**P, T**

![Graph showing mass fraction, pressure, temperature, and shock profiles over time](image-url)
Simulation vs. Experiments

Simulations

Austin 2003

H₂ + O₂ + 85% Ar
Four steps vs. single step

Mass

Pressure

Temperature
Chain-branching coefficient $a$

$a > 1$ explosion

no explosion

explosion
Reaction length

-p

\(10^{-4}\)  \(10^{-2}\)  \(10^0\)  \(10^2\)  \(10^4\)

\(L\)

\(10^0\)  \(10^1\)  \(10^2\)  \(10^3\)  \(10^4\)

explosion

no explosion

explosion

no explosion
Smoke foils
Smoke foils
Smoke foils
Kinetics: Summary

- A hierarchy of models
  - Single step
  - A few steps
  - Reduced models (10-30 steps)
  - Full kinetics
- Arguably there is use for all. None is perfect
Simulation of detonations: Issues

- Obviously kinetics and stiffness
- Size of the domain (width, length)
- Resolution especially in hot spots (Quirk)
- Grid refinement vs. parallel optimization
- Downstream BC
  - Reflective, but how? Length?
  - “overdrive” but what? P, u, T,...?
Issues (continued)

- Convergence of the inviscid model?
  - Kelvin-Helmholtz: convergence requires viscous model on the scale of the thickness of the splitter plate
  - Here: thickness of the triple point! (Mean free path, non-equilibrium?)
  - Gamezo and Oran do that.
  - If reaction fronts Rayleigh-Taylor unstable (or RM), same issue
Issues (continued)

- Length: typical 1st order termination: infinite reaction length
- Even “free propagating:” subsonic at exit
- CJ plane?
Hydrogen Safety applications  
(quite preliminary)

- Electrolyzer (with Andrei Tchouvelev)  
  (Dispersion data from Andrei)
Electrolyzer

0.06 s
Electrolyzer

0.1 s

HVOI
1.000E+00
9.347E-01
8.693E-01
8.040E-01
7.387E-01
6.733E-01
6.080E-01
5.427E-01
4.773E-01
4.120E-01
3.467E-01
2.813E-01
2.160E-01
1.507E-01
8.533E-02
2.000E-02
Electrolyzer

$0.2 \text{ s}$
Electrolyzer

0.5 s
Electrolyzer
Electrolyzer

Model: single step (Gamezo et al. 2006)
(Reaction zone not resolved anyway – Heat release is what matters)

BCs: solid walls. Ignore equipment inside

Show movies next
Electrolyzer
Electrolyzer
Electrolyzer
Electrolyzer
Electrolyzer

Initially the detonation propagates

When mixture becomes lean it fails

(Reaction front decouples from shock)

Shock weakens as it moves toward walls

Reflections: unphysical
Tunnel

Assumed 8 kg of hydrogen spilled

Cloud: half-parabolic, stoichio on top, zero hydrogen along bottom parabola (see picture)

Section: 50 m², height 5.1 m, bottom 1.5 m is vehicles so domain is 3.6 m.
Tunnel

- Ignite point
- Wall
- Symmetric boundary
- Mass fraction
- Outflow
Tunnel

Pressure gradient

Temperature gradient
Tunnel

Pressure gradient

Temperature gradient
Tunnel

- Does not look too good
- Pressure on vehicles will be high
- Would be worth looking at longer section
- Resolution may be insufficient
Summary

- Simulation of detonations
  - Not perfect
  - But not too bad either
- Situation is better than for example
  - turbulent combustion
  - hydrogen dispersion
- Much closer to actual physics
References

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