COMBUSTION: A COMPLEX SCIENCE AND AN ANCIENT BUT IMMATURE TECHNOLOGY

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PROMETHEUS
GOD OF FIRE
KAGUTSUCHI (HO-MASUBI)

“THE CREATURES OF PROMETHEUS”
BEETHOVEN’S ONLY BALLET
FUELS AND OXIDIZERS

Solid Fuels – Wood (and other biomaterials), Coal, Plastics, Metals

Liquid Fuels – Hydrocarbons, Liquid Hydrogen

Gaseous Fuels – Methane, Propane, Hydrogen

Solid Oxidizer – Ammonium Perchlorate ($\text{NH}_4\text{ClO}_4$)

Liquid Oxidizer - Liquid Oxygen

Gaseous Oxidizer – Air, Oxygen, Fluorine

*Solids and Liquids can occur in bulk or as particles (droplets or dust).*
MEASURES

- PERFORMANCE
  * Fuel consumption rate / Power (Thrust)
  * Miles / Gallon of fuel
  * Power (Thrust) / Air flow rate
  * Power (Thrust) / Engine weight

- EMISSIONS
  * Parts per million of pollutant

- ECONOMY
  * Fuel consumption rate / Power (Thrust)
  * Capital costs: research, development, and manufacture
### THE FOUR ELEMENTS

<table>
<thead>
<tr>
<th>Empedocles</th>
<th>Fire</th>
<th>Air</th>
<th>Water</th>
<th>Earth</th>
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<tbody>
<tr>
<td></td>
<td><img src="image1.png" alt="Pyramid" /></td>
<td><img src="image2.png" alt="Octahedron" /></td>
<td><img src="image3.png" alt="Icosahedron" /></td>
<td><img src="image4.png" alt="Cube" /></td>
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<td>Plato:</td>
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<td>Platonic Solids</td>
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<td>with Triangles</td>
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<td>Aristotle</td>
<td><img src="image5.png" alt="Hot &amp; Dry" /></td>
<td><img src="image6.png" alt="Hot &amp; Wet" /></td>
<td><img src="image7.png" alt="Cold &amp; Wet" /></td>
<td><img src="image8.png" alt="Cold &amp; Dry" /></td>
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> The Ancient Chinese, Hindu, and Buddhists each had three to five elements; fire was always one of them.

> Neither Plato or Aristotle were exactly on the mark but the world unfortunately went down the “touchy, feely” path of Aristotle rather than the mathematical path of Plato.
> Began in Alexandria in early A.D. period.
> Alchemists can broadly include magicians, mystics, and fakers. We will emphasize early chemists, biochemists, and metallurgists.
> Many pursued Aristotle’s Theory of Transmutation, e.g. attempt to convert lead to gold.
> Fire was the “element of transformation.”
> Fire was also the first chemical reaction that man could produce and control.
IMPORTANT 18TH - CENTURY DEVELOPMENTS

> Georg Ernst Stahl, early 1700s -- All combustible materials give off “phlogiston” when burning; air absorbs phlogiston.
> Joseph Black, 1750s -- Identified carbon dioxide.
> Henry Cavendish, 1760s -- Identified hydrogen and thought it was pure phlogiston.
> Carl Scheele and Joseph Priestly, 1770s -- Independently discovered oxygen; Priestly thought air was oxygen plus phlogiston and oxygen absorbed phlogiston during combustion.
> Antoine Lavoisier, late 1700s -- discovered that the weight of the reactants of combustion equals the weight of products: law of conservation of mass. During combustion, oxygen was removed from the surrounding air. (He got it right! The phlogiston theory died.)
HENRI LOUIS LE CHATELIER (1850 – 1936)

- Most famous for Chemical Equilibrium Principle
- Unusually good genes for a chemist
  (His father was an engineer)
- Unusually well educated for a chemist
  (He had a degree in mining engineering)
- Known for connecting theory and practice
  * Synthesis of Ammonia  * Setting of Cement
  * Steel and Alloys  * Combustion and Explosions
- Technology did not wait for him:
  James Watts (1736-1819) ; Nikolaus Otto (1832-91)
“Wilbur and I were busy in completing the design of the machine itself. The preliminary tests of the motor having convinced us that more than 8 horse power would be secured, we felt free to add enough weight to build a more substantial machine than we had originally contemplated.”
Current technology does not deliver sufficient energy nor power density in the size needed for autonomy.
COMBUSTION APPLICATIONS

- ACCIDENTAL FIRE
- SPACE HEATING, COOKING, LIGHTING
- RELIGION
- INCINERATION
- METALLURGY, KILNS
- WEAPONS
- BLASTING
- ENGINES: POWER & PROPULSION
PREMIXED FLAME

This type of flame occurs in accidents, Bunsen burners, and spark ignition engines.
This type of flame occurs in accidents, oil or coal furnaces, Diesel engines, gas-turbine engines, rocket engines, and incinerators.
Combustion Science also attracts material scientists to the challenge of material behavior in very hostile (hot, oxidizing) environments.
Combustion is a heat addition process; chemical energy is converted to thermal energy (heat) via an exothermic oxidation process; e.g.,

\[
\text{CH}_4 + 2 \text{ O}_2 + 7.52 \text{ N}_2 \rightarrow \text{CO}_2 + 2 \text{ H}_2\text{O} + 7.52 \text{ N}_2 + \text{heat}
\]

Sometimes the heat from combustion is needed for the application; more often we want work (power or propulsion). So the heat must be converted to mechanical energy.

Entropy is a measure of disorder. The greater the disorder, the lower the work that can be obtained from a given amount of heat. So, we try to convert chemical energy to thermal energy (add heat) with a minimal increase in entropy (disorder).
The Second Law of Thermodynamics says that the increase in entropy becomes lower when heat is added at higher temperature: \[ \Delta S = \frac{Q}{T} \]

At higher pressures, the temperature will be higher and therefore \( \Delta S \) will be lower. Consequently, more work can be obtained.

One practical temperature limitation results from a need for materials integrity; confinement must be maintained. No deterioration, softening or melting is allowed.

Another limitation occurs due to chemical dissociation. Some energy remains in chemical form because bonds break at high temperature:

\[
\text{CH}_4 + 2\text{O}_2 + 7.52 \text{N}_2 \rightarrow a \text{CO}_2 + b \text{CO} + c \text{H}_2\text{O} + d \text{H}_2 + e \text{O}_2 \\
+ f \text{O} + g \text{H} + h \text{N}_2 + i \text{NO} + j \text{N} + k \text{C} + ----
\]
SCALAR EQUATIONS

\[ \rho \frac{\partial h}{\partial t} + \rho \mathbf{u} \cdot \nabla h - \nabla \cdot (\lambda / c_p) \nabla h = \rho \dot{w}_F Q + \frac{\partial p}{\partial t} \]

\[ h = \sum_i Y_i \int_{T_{ref}}^{T} c_{pi} (T') dT' = \sum_i Y_i h_i = \int_{T_{ref}}^{T} c_p (T') dT' \]

\[ \rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{u} \cdot \nabla Y_i - \nabla \cdot (\rho D \nabla Y_i) = \rho \dot{w}_i ; \quad i = F, O, P \]

- \( h \) is enthalpy, a measure of thermal energy.
- \( Y_i \) is the fraction of mass per unit volume (density) associated with species \( i \).
Equations of Fluid Motion

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) + \frac{\partial}{\partial z} (\rho w) &= 0 \\
\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \rho w \frac{\partial u}{\partial z} + \frac{\partial p}{\partial x} &= \frac{\partial}{\partial x} \left[ \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right) \right] \\
&\quad + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right]
\end{align*}
\]

\[
\begin{align*}
\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \rho w \frac{\partial v}{\partial z} + \frac{\partial p}{\partial y} &= \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial v}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] \\
&\quad + \frac{\partial}{\partial z} \left[ \frac{2}{3} \mu \left( \frac{\partial v}{\partial z} - \frac{\partial u}{\partial x} - \frac{\partial w}{\partial y} \right) \right]
\end{align*}
\]

\[
\begin{align*}
\rho \frac{\partial w}{\partial t} + \rho u \frac{\partial w}{\partial x} + \rho v \frac{\partial w}{\partial y} + \rho w \frac{\partial w}{\partial z} + \frac{\partial p}{\partial z} &= \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] \\
&\quad + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ \frac{2}{3} \mu \left( \frac{\partial w}{\partial z} - \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) \right]
\end{align*}
\]
FLUID DYNAMIC PHENOMENA

- Shock waves -- increase pressure, temperature and reaction rates, important in detonations.

- Turbulent fluctuations -- enhance mixing rates and thereby accelerate combustion rates, also enhance heat losses.

- Flow separation – allows jet formation with associated penetration, wake or cavity recirculating flow formation which protects flame in its ignition region.
Shockwave forms in high speed (supersonic) flow.
- Blunt object creates aft recirculation zone in the near wake.
- Recirculation zones provide protected low speed regions for ignition and flameholding.
- Wake can become turbulent at high speeds, enhancing mixing.
The fluid leaves (separates from) the wall of the tube to form a jet. Then, the laminar (smooth) flow transitions to turbulent (rough) flow. Jets allow penetration of one fluid into another. Turbulence enhances mixing rates.
MULTIPLE & DISPARATE LENGTH AND TIME SCALES

- Chemical times, usually fast, different scales for different reactions. Reaction zone size.


- Flow or residence times. Chamber size.

- Turbulent eddy length and time scales.

- Multiple and disparate lengths and times present challenges to measurement science.

- Multiple and disparate lengths and times present challenges to computational science.
NON-INTRUSIVE MEASUREMENTS IN HOSTILE ENVIRONMENTS

Coherent Anti-Stokes Raman Spectroscopy (CARS)

Courtesy of Prof. D. Dunn-Rankin
EXAMPLES OF SCIENTIFIC AND TECHNOLOGICAL CHALLENGES

> Fuel Droplets and Sprays - *diffusion flames*
  -- individual droplet behavior at subcritical thermodynamic conditions
  -- individual droplet behavior at supercritical thermodynamic conditions
  -- spray behavior in a combustor
  -- formation of a spray, atomization

> More Efficient Engines -- Turbine Burner

> More Compact Engines -- Liquid-Film Combustors

> Fire Safety -- Flame Spread Above Liquid Fuels
  -- at earth gravity conditions
  -- in spacecraft conditions
CONVECTIVE DROPLET VAPORIZATION

Internal circulation enhances heating and vaporization.
Polydisperse spray injected into recirculating, turbulent reacting gas.
CRITICAL THERMODYNAMIC CONDITIONS

At high pressures and temperatures, there is no distinction between phases.
Ambient gas begins at supercritical state but cold droplet is subcritical. As the droplet is heated, the critical surface moves towards the droplet surface. When the surface is reached, distinction between the phases disappears.
OXYGEN DROPLET VAPORIZING IN HYDROGEN GAS
Existing Experimental Investigations of Liquid-Phase-Modulated Sprays

Sources: I.-P. Chung et al. 1998 (Conical Sheet); Brenn, Rensink & Durst 2000 (Fan Sheet)
SPRAY ATOMIZATION

Liquid sheet is injected in a hollow “conical” form to maximize surface area and rate of droplet formation. 

Courtesy of Dr. C. Mehring
TURBOFAN CYCLE
Flow accelerates through transonic range and turns; streamwise and transverse accelerations can be $O(10^5 \ g)$.
Burning in the turbine has advantage in a temperature-limited system; many stator burners approach continuous burner.
M = 2, \; T_4 = 1500 \text{ K}, \; T_6 = 1900 \text{ K}
Fuel injection into curved, convergent-divergent channel
Typical of turbine blade passage. Mixing and reaction occur in a diffusion flame while flow turns and accelerates at about $10^5$ g.
LIQUID-FILM COMBUSTOR: Conceptual Design

Swirling air flow

Flame

Liquid Film

Streamlines

Recirculation Caused by Strong Swirl
LIQUID-FILM COMBUSTOR

- Methanol/methane /air and heptane/air burns internally
- Pure gas flame not internal
- Swirl control

Pyrex combustor
NASA MICROGRAVITY FACILITIES

> Space Shuttle
> Sounding Rockets
> KC-135
> Drop Towers
NASA Microgravity Program

FLAMES ABOVE LIQUID FUELS

![Diagram of flame spread process with labels for Buoyant Airflow, Forced Airflow, Recirculation Cell, heated region, Surface-tension-driven flow, return flow in finite pool, and bottom of pool.]

Courtesy of Dr. H.D. Ross, NASA Glenn
Thank you for your attention.
Power and Energy Density

- **Energy Density (Whr/kg)**
  - Hydrocarbon fuel > 10000 Whr/kg
  - Solar -- 100 W/kg

- **Power Density (W/kg)**
  - 10000
  - 1000
  - 100
  - 10
  - 1

- **Full size combustion engines**: 1000 hr
- **Combustion**:
  - Model airplane engine: 6 min
  - Hummingbird and insect metabolism: 3.6 sec
  - Mini-diesel: 36 sec
- **Fuel cell**: 10 hr
- **Lead acid battery**: 100 hr
- **Rechargeable lithium**: 100 hr
- **Primary lithium**: 100 hr
- **Human metabolism**: 1 hr

- **Courtesy of Prof. D. Dunn-Rankin**
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