# Are There Practical Approaches For Achieving the Theoretical Maximum Engine Efficiency?



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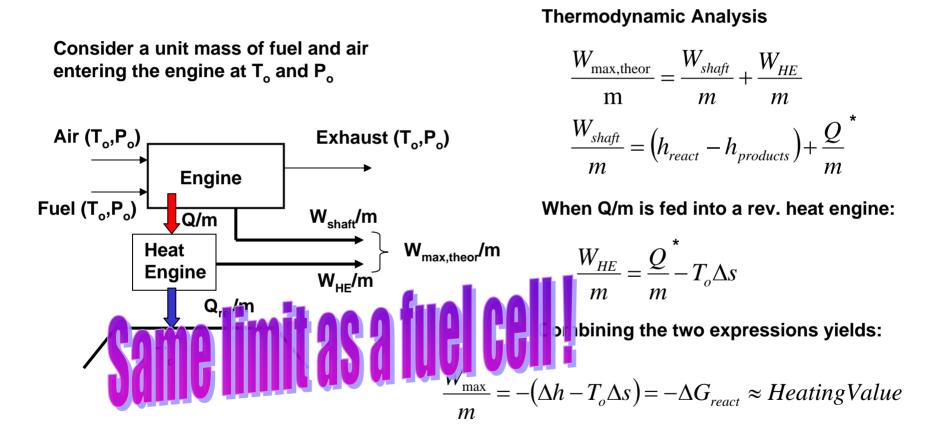
– Ron Graves and Stuart Daw

- Colleagues of the "Thermodynamics Discussion Group"
  - Oak Ridge National Labs,
  - Roy Primus, Jerry Caton, John Clarke

### **Two Questions:**

- What is the maximum theoretical efficiency that can be achieved with an internal combustion engine?
- What is the practical maximum efficiency that can be achieved with an internal combustion engine?

## **Maximum Theoretical Efficiency**



\*Realize that because the system changes, these two heat transfers will have opposite signs

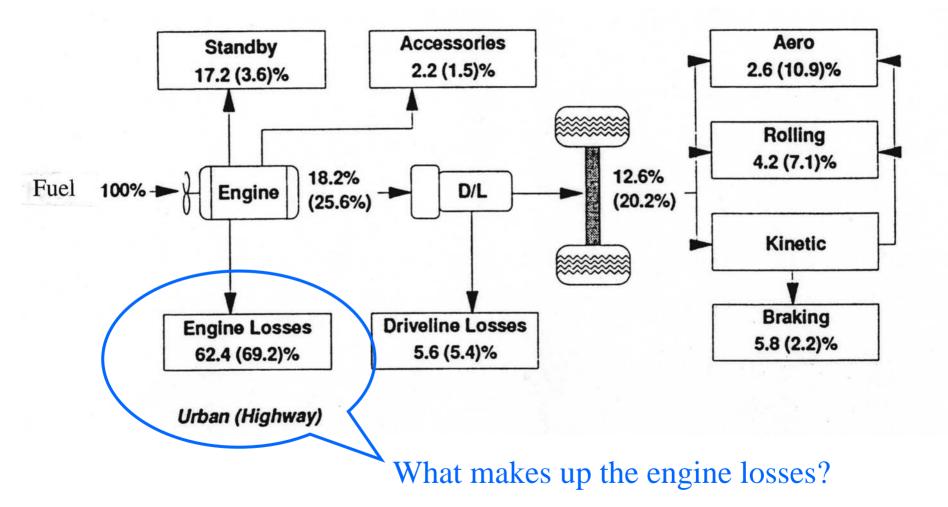
# **Determining Practical Limitations**

#### **Use the 2nd Law to Assess Losses**

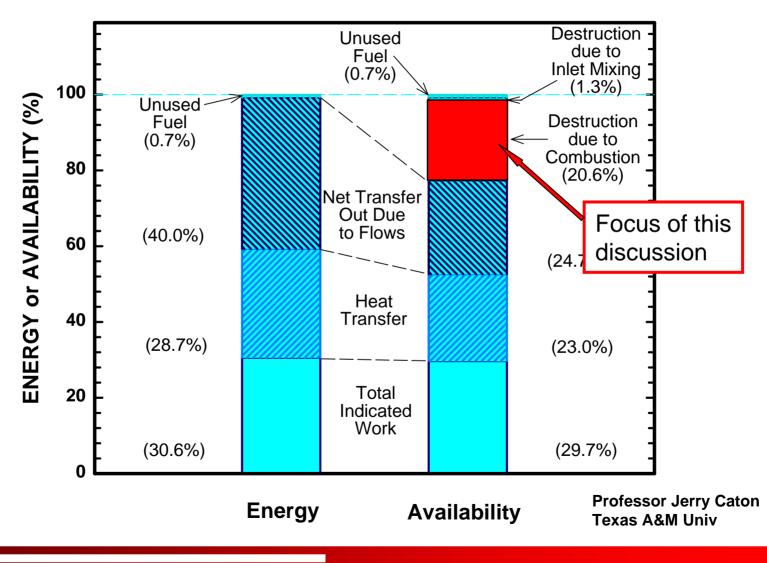
$$\frac{dS}{dt}\Big|_{system} = \frac{Q}{T} + \sum \dot{m}_{in} s_{in} - \sum \dot{m}_{out} s_{out} + \dot{S}_{producted} : \qquad \dot{W}_{lost} = T_o * \dot{S}_{produced}$$

- Three thing can change the entropy of a system:
  - Heat transfer
  - Mass transfer
  - IRREVERSIBILITIES!

#### **Energy Distribution in a Mid-Size Car (PNGV)**



#### **Overall Energy and Availability Values**



Classification of Combustion Irreversibilities (Dunbar and Lior)

- Diffusion process, where the oxygen and fuel molecules are drawn together
- Chemical reaction
- Internal-thermal energy exchange, where product molecules "share" their kinetic energy with their neighbors
- Mixing process whereby the system constituents mix uniformly

## Example

W.R. DUNBAR AND N. LIOR

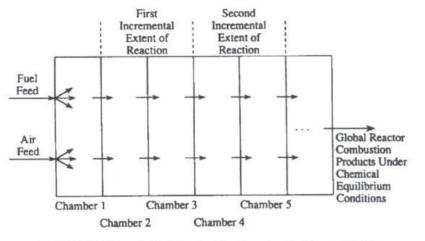
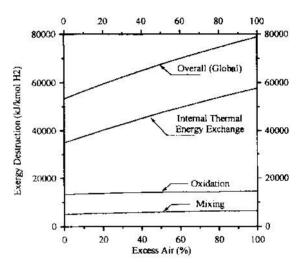


FIGURE 8 Hypothetical Combustion Chamber for Process Path 2.



Hydrogen Combustion Subprocess Exergy Destruction vs. Excess Air, Path 2.

- Fuel and air mix
- A portion reacts to completion adiabatic flame temperature
- These hot products heat the unreacted mixture
- The process repeats until the mixture reaches the autoignition temperature

#### **Losses in Combustion**

Rate of lost work = 
$$T_0 * \overset{\bullet}{S}_{produced} = T_0 * \sum_{j=1}^{\tau} \sum_{i=1}^{r} \left( -\frac{\nu_i^{(j)} \mu_i}{T} \right) * \overset{\bullet}{\xi}_j$$

 $\mu_i$  = chemical potential of i-th constituent

 $v_i^{(j)}$  = i-th stoichiometric coefficient of the j-th reaction mechanism

 $\tau$  = number of reactions, r = number of species

with: 
$$\xi_j = k * [N_i]^{\nu_i} * [N_k]^{\nu_k}$$
  
where:  $k = B * T^n * \exp\left(\frac{-E_A}{\overline{R}T}\right)$ 

# How does one reduce the loss of availability during combustion?

Present combustion engines seem to maximize this loss.....\*

- Big temperature gradient Reactants → Products
- Far from equilibrium
  - Dissociation of species
  - Energy stored in molecular states difficult to convert to work
  - Composition "frozen" during rapid expansion

\*outcome of focus on Otto cycle

Possible corrective routes

- •Raise the temperature of reaction closer to reversible upper limit
- •Change the chemistry to lower the equilibrium temperatures
  - •Weak mixtures
  - •Staged reactions (e.g.reforming)
  - •New ideas? Fuels?
- •Must capture, not exhaust

# The Mechanisms of Loss Can Be Explained as Follows:

- The availability destruction is directly proportional to the rate at which the chemical reactions are taking place.
  - Explains the efficiency characteristics of a fuel cell
- The availability destruction is directly related to the affinity of the reactions that are occurring.
- The availability destruction appears to be inversely related to the temperature at which the reactions are taking place.

#### Approaches to Reduce Combustion Irreversibilities

- Slowing down the chemical reactions
- Choosing fuels or establishing stoichiometries such that the chemical reactions have lower affinity
- Raising the temperature at which the reactions occur.

# If It Only Were That Simple

- Raising the temperature will have offsetting effects
  - Higher temperatures will increase the rate of chemical reaction, which increases the rate of availability destruction. This will offset the reduction in availability destruction rate caused by the temperature in the denominator
- The total availability destruction will be the integration of the rate of destruction over the duration of the combustion process
  - Thermodynamics tells us that the total availability destruction will be determined by the end states of the chemical reaction process
    - Lower rates integrated for longer combustion durations will result in the same availability destruction as higher rates integrated for shorter time periods (If the end states are the same.)
- To reduce the total availability destruction during combustion, the end states need to be altered.

## **Question:**

 Is the large availability destruction currently experienced in our engine combustion processes the result of very different rates at which the chemical reaction takes place compared to the rate at which work is extracted?

#### Conceptual Ideas and Resulting Characteristics

- Achieve energy release with "volumetric" reactions that are locally slow but keep the integrated mass burn rate high
  - Low temperature combustion low emissions of NOx and particulate matter
- More closely match the rate of energy release with the rate at which work is being extracted
  - Changing the end states
  - Interesting anecdotal studies of piston variable piston motion for maximum efficiency

# **Possible Implications and Issues**

- Irreversibilities of reaction may decrease at the expense of lower power
- If this occurs, the available energy would be transferred to the exhaust, instead of being destroyed.
  - Exhaust energy recovery would be critical to the success of such a process
- Identifying the trade-offs between lower availability destruction during combustion with the desire for high power density

Current Approaches to Reduce Emissions May Also be Moving Toward Lower Combustion Losses

- Do away with flame propagation as the means of energy release
  - HCCI, MK, CAI, PCCI, etc.
  - Very Early Diesel Injection
    - Fuel modifications low cetane number with low octane number
  - Mixing controlled autoignition
    - Sophisticated injection systems matched to the thermodynamic states of the cylinder to establish distributed reaction energy release
- Low Temperature Combustion

# **Conceptual Engine ?**

- Very high compression ratio CR>50
  - Peak pressure is achieved at TDC of motoring
- Injection always occurs aTDC (MK like)
  - Load can be controlled by the quantity of fuel injected and the expansion ratio allowed (injection timing)
- Mixing needs to be very fast, or fuel needs to be special, low cetane number and low octane number (naptha, light kerosene, cycloparaffins...)
- Energy release (combustion) needs to occur slowly (burn rate is obtained via volumetric reaction, with simultaneous "heating" of "inerts"), and be more closely matched by the rate at which the piston is expanding

# Closure

- Lowering fuel consumption is becoming an increasingly important metric
- Chemical reaction irreversibilities represent a significant impediment to maximizing powerplant system efficiency (both IC engines and fuel cells)
- If irreversibilities of combustion can be reduced, how will the availability partitioning of the engine system be affected?
- Total powerplant system energy utilization and optimization will be an important perspective from which to evaluate total fuel conversion efficiency
- Perhaps second law analysis will be useful afterall.