Format of the exam

90 minutes allowed. The midterm exam will be open book to the extent of lecture notes, your personal notes, homework sets and solutions and the (optional) textbooks by Heywood, Mattingly and Turns.

Material covered

The exam may cover any material through lecture 5. This includes:

- Introduction
  - Classifications of IC engines
  - Advantages and disadvantages of each type
  - Alternatives to IC engines and hydrocarbon fuels
  - History and evolution
  - Where room for improvement is and isn’t

- Fuels and combustion
  - Fuel types
  - Chemical thermodynamics
    - Balancing chemical reactions (stoichiometry, fuel mass fraction, equivalence ratio)
    - 1st Law of Thermodynamics for a chemically reacting system
      - Heating value
      - Adiabatic flame temperature
    - 2nd Law of Thermodynamics for a chemically reacting system
      - Degrees of Reaction Freedom (DoRFs)
      - Chemical equilibrium
      - Isentropic compression/expansion
        - Entropy of a gas mixture
        - Frozen and equilibrium expansion
  - Combustion
    - Chemical reaction rates
      - Law of Mass action
      - Arrhenius term – \( e^{\frac{E}{\mathcal{R}T}} \) – responsible for extreme sensitivity of reaction rates to temperature whenever \( E/\mathcal{R}T >> 1 \) (say 5 or more)
    - Premixed flames
      - Deflagrations
        - Burning velocity – depends mostly on \( T_{ad} \)
        - Effects of turbulence
      - Homogeneous reaction – depends mostly on \( T_c \)
    - Non-premixed flames
      - Droplets
      - Gas-jets

- Pollutant formation and remediation
o Which emissions are bad?
  • Atmospheric photochemical cycle
  • Greenhouse effect
  • Emissions regulations
o Emissions are a non-equilibrium phenomenon – if everything went to equilibrium there would be no emissions!
  • \( \text{NO}_x \)
    • Thermal or Zeldovich NO
      o Formed at high \( T \) - very high activation energy process
      o Slow time scale – forms in products, not in flame itself
      o Lean mixtures (surplus \( \text{O} \)) favors \( \text{NO} \) formation
      o Rich and cool better (no excess \( \text{O}_2 \)), low temperatures
    • Prompt \( \text{NO} \)
      o Formed in the flame
  • \( \text{CO} \), unburned hydrocarbons (UHC), formaldehyde (\( \text{CH}_2\text{O} \))
    • Formed due to incomplete combustion or “trapped” fuel (e.g. crevice volumes)
    • High \( T \) and excess \( \text{O}_2 \) needed to minimize emissions – oxidize \( \text{CO} \) to \( \text{CO}_2 \) and \( \text{UHC}/\text{CH}_2\text{O} \) to \( \text{CO}_2 \) and \( \text{H}_2\text{O} \)
o Soot
  • Premixed
    • Only formed in rich mixtures, in combustion products
    • Critical equivalence ratio
    • More soot at lower temperatures because soot formation must compete with oxidation
    • Doesn’t depend on fuel structure because fuel is destroyed in flame front – molecules have to reassemble in combustion products
  • Nonpremixed
    • Forms on rich side of flame front
    • More soot at higher temperatures because no competition between formation and oxidation
    • Depends on fuel structure because fuel molecules not destroyed by flame front before soot can form
o Cleanup
  • Premixed - \( \text{CO} \), UHCs main concern
    • Burn at stoichiometric with EGR to reduce flame temperature
    • 3-way catalyst, oxidizing for \( \text{CO} \), UHC, \( \text{CH}_2\text{O} \), reducing for \( \text{NO} \)
  • Nonpremixed – \( \text{NO} \), soot main concerns
    • Can’t use 3-way catalyst since mixture is lean overall – won’t reduce \( \text{NO} \)
    • Need particulate traps for soot, Selective Catalytic Reduction for \( \text{NO} \)
A previous year’s first midterm exam (should look familiar…)  (average was 68.8/100)

Problem #1 (chemical thermodynamics) (30 points total, 5 points each part)

It is proposed to “reform” propane (C₃H₈) by burning it in air under very rich conditions so that the products are CO, H₂ and N₂ rather than the usual CO₂, H₂O and N₂. (This CO and H₂ mixture will then be used in a fuel cell rather than an engine, but that’s not part of this problem.)

<table>
<thead>
<tr>
<th></th>
<th>C₃H₈</th>
<th>O₂</th>
<th>N₂</th>
<th>CO</th>
<th>H₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δh°ᵣ (kJ/mole)</td>
<td>-104.70</td>
<td>0</td>
<td>0</td>
<td>-110.54</td>
<td>0</td>
</tr>
<tr>
<td>Molecular mass (g/mole)</td>
<td>44</td>
<td>32</td>
<td>28</td>
<td>28</td>
<td>2</td>
</tr>
</tbody>
</table>

a) Write down the stoichiometric reaction, i.e., find a, b, c and d for the reaction

1 C₃H₈ + a air → b CO + c H₂ + d N₂

b) What is the stoichiometric mass fraction (f) of this propane-air mixture with this set of assumed products (CO, H₂, N₂)?

c) What is the heating value of propane (in J/kg) with this set of assumed products?

d) What are the molecular mass (in g/mole) and gas constant (in J/kgK) of the product mixture?

e) What is the Cp of the product mixture if the mixture-averaged specific heat ratio γ = 1.35?

f) What is the constant-pressure adiabatic flame temperature of this mixture if the reactants are at 298K?

Problem #2 (30 points total)

Consider a mixture of 30 mole % H₂O and 70 mole % He (helium) at 2000K and 3 atm. Assume that the H₂O dissociates into H₂ and O₂ but no other products of dissociation (e.g. H, OH, O) occur. (Helium does not dissociate and thus does not participate in any equilibrium reactions.)

<table>
<thead>
<tr>
<th></th>
<th>H₂</th>
<th>O₂</th>
<th>He</th>
<th>H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δh°ᵣ (kJ/mole)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-241.83</td>
</tr>
<tr>
<td>Molecular weight (g/mole)</td>
<td>2</td>
<td>32</td>
<td>4</td>
<td>18</td>
</tr>
<tr>
<td>K (equilibrium constant) at 2000K</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>3492</td>
</tr>
</tbody>
</table>

a) (15 points) Write down ALL relations needed to solve for the mole fractions of H₂O, H₂, and O₂ and He (that means you need as many equations as unknowns)

b) (15 points) Solve these equations. Hint: it’s not as bad as it seems; you can simplify the algebra a lot since X₃H₂ << 1 and X₀₂ << 1.

Problem #3 (40 points total, 5 points each part)

Ronney Oil and Gas Co. has invented a new fuel, called PDR™, that has all the same chemical, thermodynamic and transport properties as octane. The only difference between octane and PDR™ is that PDR™ has 10% lower activation energy for all chemical reactions involving the fuel molecule (octane or PDR™). If PDR™ were used instead of octane, how would each of the following combustion properties change? In particular, would the property increase, decrease or remain the same and by less than, more than, or exactly 10%?

a) Constant-pressure adiabatic flame temperature of a stoichiometric mixture

b) Laminar burning velocity of a stoichiometric mixture

c) Time for homogeneous explosion in a stoichiometric mixture

d) Burning rate of a fuel droplet burning in air

e) Rate of thermal NO formation immediately downstream of a stoichiometric premixed flame

f) Amount of unburned hydrocarbon emission from a premixed-charge engine.

g) Amount of soot formation in a rich premixed flame (think carefully about this one!)

h) Amount of soot emission from a non-premixed flame.