Thermophysical Properties of Hydrogen as an Energy Carrier

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Presentation Outline

- Our energy future
- Hydrogen production, storage, and use
- Role of thermophysical properties in design
- Status of current property data and formulations
- Future research
Our Energy Future

- World energy demand increasing in China, India and other developing countries
- Middle Eastern countries controlling the supply of oil
- Gasoline prices at the pump -- $3.00 per gallon or more
- President Bush’s 2003 Hydrogen Fuel Initiative
  - $289.5 million requested for FY 2007
Hydrogen Implementation

- Vancouver Hydrogen highway infrastructure
  - In operation by 2010 Winter Olympics
Hydrogen Implementation

- California Hydrogen highway infrastructure
  - 13 existing stations
  - 170 stations in operation by 2010
  - Over 60 cars in operation
What’s Hydrogen?

- Most abundant element in the Universe
  - 75% of all mass, 90% of all atoms
- Colorless, odorless, tasteless gas
- Diatomic molecule
- An energy carrier or fuel
- Does not exist in pure form on earth
The Hydrogen Supply

- Generation
  - Fossil Fuels
  - Electrolysis
  - Nuclear
  - Biological
  - Thermo-chemical

- Storage and Distribution
  - Compressed gas
  - Cryogenic liquid
  - Slush
  - Absorbed

- Sale and Usage
  - Internal Combustion
  - Fuel Cells
Supplier and Consumer Questions

- Safety?
- Efficiency?
- Costs of buying and selling?
- **Answer:** Well designed systems.
Design of Hydrogen Systems

- Require accurate properties of hydrogen
- Custom experimental measurements not practical
- All thermodynamic properties from an Equation of State (EOS)
- All transport properties from a separate formulation
- EOS and transport formulations model published experimental data
EOS Formulation

- EOS are created by fitting experimental data
- Data maps show existing experimental data
- Temperature scales must be updated
- Equations are limited by the range and accuracy of experimental data

Normal Hydrogen Data Map P-v-T
EOS Formulation

- Deviation plots compare EOS to experimental data
- Deviations represent flaws in the EOS
- Uncertainty based on EOS deviations from experimental data

\[
\text{% deviation in density} = 100 \times \frac{\rho_{\text{data}} - \rho_{\text{calc}}}{\rho_{\text{data}}}
\]
Standard Hydrogen EOS Accuracies

- Hydrogen standard EOS from 1982
- Methane standard EOS from 1991 has better accuracies

<table>
<thead>
<tr>
<th>Property</th>
<th>Estimated Uncertainty in Normal Hydrogen and Methane EOS</th>
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<tbody>
<tr>
<td></td>
<td>Liquid H₂</td>
</tr>
<tr>
<td>Density</td>
<td>0.1%</td>
</tr>
<tr>
<td>Heat Capacity</td>
<td>3%</td>
</tr>
<tr>
<td>Speed of Sound</td>
<td>2%</td>
</tr>
<tr>
<td>Viscosity</td>
<td>4-15%</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>1-10%</td>
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</tbody>
</table>
Importance of Accuracy

- U.S. used 440 million gallons of gasoline daily in 2004
  - 1 gallon of gasoline ≈ 1 kg of hydrogen
  - Gasoline $2.50 per gallon and fluctuating
  - 0.2% uncertainty in density calculation
  - $2.2 million discrepancy in gross product sale every day

\[
\text{(440 million gallons gasoline)} \times \$2.50 = \$1.1 \text{ billion}
\]

\[
\text{($1.1 \text{ billion})} \times (0.002) = \$2.2 \text{ million discrepancy}
\]
Standard Hydrogen EOS Limits

- Upper temperature limit of 400 K
Hydrogen: 2 different molecules

Molecular Hydrogen – H₂

- orthohydrogen
  - higher energy state
  - cannot exist in pure form

- parahydrogen
  - lower energy state
  - can exist in pure form

Normal
3 : 1
Equilibrium Hydrogen

- Percentage of parahydrogen in equilibrium mixture
- Predicted by quantum mechanics and statistics
Modeling the Hydrogen Forms

- The different forms have different thermophysical properties
  - Ideal gas behavior predicts differences
- Two different EOS exist
  - Parahydrogen EOS (pure fluid)
  - Normal hydrogen EOS (treats normal hydrogen mixture as pure fluid)
- No mixture EOS exists for parahydrogen and orthohydrogen
Storage Behavior

- Conversion between forms causes energy change
- Energy change greater than the latent heat of vaporization
CATS Research

- Survey of published hydrogen properties
  - Over 200 hydrogen property papers identified
- Status of standard formulations for both thermodynamic and transport properties
- An orthohydrogen EOS
  - Mix orthohydrogen with parahydrogen
- Updated property formulations
Conclusions

- Accuracy of hydrogen EOS must be increased
- New hydrogen EOS must be accurate at high and cryogenic temperatures
- Hydrogen mixture EOS must be created
Questions?

Source: General Motors Corporation