## NIST Property Models and Data Support the Transition to Hydrogen as a Transportation Fuel

NIST work on the properties of hydrogen has been incorporated into two new standards that will support the development of hydrogen as a fuel in vehicle applications. A new, simplified equation for the density of hydrogen gas was developed for the draft SAE (Society of Automotive Engineers) procedure J2572. The NIST REFPROP equations for the thermodynamic and transport properties of hydrogen form the basis for the new ASTM International Standard D7265-06. We have also begun an experimental program, which will generate the data necessary to develop improved models for hydrogen and hydrogencontaining mixtures.

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One of the challenges in the use of hydrogen in vehicle applications is the seemingly trivial matter of measuring fuel consumption. Consumers and industry are accustomed to the high accuracy that is easily achievable by the volumetric metering of gasoline and other liquid fuels. But hydrogen, used either as a compressed gas or a cryogenic liquid, presents significant metering challenges. Vehicle manufacturers have proposed a number of different protocols and algorithms for their hydrogen-fueled vehicles, and the EPA approached NIST to help provide a baseline for an appropriate standard. To evaluate the consumption of gaseous hydrogen fuel in motor vehicles, determination of the temperature and pressure before and after usage within a storage tank of known, and essentially fixed, volume is one of three methods recognized in the SAE draft procedure J2572 "Recommended Practice for Measuring the Fuel Consumption and Range of Fuel Cell Powered Electric and Hybrid Electric Vehicles Using Compressed Gaseous Hydrogen." Compared to the alternative methods of continuously metering the flow of hydrogen to the fuel cell or weighing the fuel tank before and after a test, the use of pressure, volume, and temperature measurements has the potential to be the most robust and economical method in terms of instrumentation costs and ongoing personnel test resources, as well as for measurement precision, repeatability, accuracy, and lab-to-lab reproducibility. The EPA National Vehicle Fuel and Emission Laboratory (NVFEL) is currently evaluating this method for fuel cell (FC) and internal combustion (IC) engines.

In support of SAE J2572, we developed a new equation for hydrogen gas densities using a truncated virial-type equation for the density of hydrogen in terms of pressure and temperature. The new equation reproduces the available experimental data to within 0.2 % (combined uncertainty with a coverage factor of two) and is recommended for use

over the temperature range 220 to 400 K at pressures up to 45 MPa. This equation will standardize calculations of hydrogen fuel consumption in vehicles, and represents an initial facet of the NIST effort to help build the infrastructure for a hydrogen-based economy.

In a related effort, the hydrogen property values from the NIST REFPROP database form the basis for the new ASTM International standard D7265-06 "Standard Specification for Hydrogen Thermophysical Property Tables." This standard specification was written by NIST staff who also led the specification through the approval process within ASTM Committee D03 on Gaseous Fuels.

The SAE and ASTM documents (as well as the hydrogen properties in the current version of REFPROP) are based on an existing NIST Standard Reference Data formulation dating from 1982. This formulation is "old-fashioned" by current standards and must certainly be improved, but the immediate needs of industry demanded that we provide interim data. In anticipation of the development of more modern equations of state and property formulations, we have collaborated with researchers from the University of Idaho to survey the available thermophysical properties data for hydrogen over the entire fluid surface (not just the compressed gas). This survey will help to identify regions where additional data may be needed to support new applications.

We also initiated in FY'06 what is expected to be an ongoing experimental effort on hydrogen systems with measurements of the heat capacity and thermal conductivity of a methane plus hydrogen blend. The measurements extended from 140 to 350 K with pressures up to 20 MPa. This blend is used as a fuel, but the primary motivation was to provide data for developing models of hydrogen-containing mixtures.

The correlations developed this year will satisfy immediate needs of our customers, and will be disseminated through standard reference databases, such as NIST REFPROP.

Before this NIST effort, there was no generally accepted industry-wide method of calculation for hydrogenfueled vehicles.

*Future Plans:* A significant initiative on "codes and standards for the hydrogen economy" is being considered for funding in the FY'07 NIST budget. Under this initiative, we would significantly expand our experimental efforts on hydrogen and hydrogen-containing mixtures, which would be important in the production of hydrogen (e.g. process streams in coal gasification) or as fuels in their own right (e.g. hydrogen-methane blends). We will develop modern equations of state and other property formulations for hydrogen. We will work to satisfy the immediate data needs of industry, delivering interim data and models when necessary, while working towards the broader, long-term goal of developing comprehensive, high-accuracy property models for hydrogen and hydrogen-containing systems.

## **Publications**

D7265-06 Standard Specification for Hydrogen Thermophysical Property Tables, ASTM International, 2006.

E. W. Lemmon, M.L. Huber, D.G. Friend, and C. Paulina, "Standardized Equation for Hydrogen Gas Densities for Fuel Consumption", Paper 2006-01-0434, Proceedings SAE World Conference, April 3-6, 2006 Detroit, MI

R.T Jacobsen, J.W. Leachman, S.G. Penoncello, and E.W. Lemmon, "Current Status of Thermodynamic Properties of Hydrogen", Int. J. Thermophysics, submitted Aug 2006.

J.W. Leachman, R.T Jacobsen, S.G. Penoncello, and M.L. Huber, "Current Status of Transport Properties of Hydrogen", Int. J. Thermophysics, submitted Aug 2006. **Project Team:** E.W. Lemmon, M.L. Huber, D.G. Friend, D.G. Archer, M.O. McLinden, R. Perkins, J. Magee, (Physical and Chemical Properties Div.); R.T Jacobsen and J.W. Leachman (University of Idaho); C. Paulina (EPA)

## Figure 1.

Hydrogen fuel-cell powered vehicle undergoing tests of fuel economy.

