

# PROJECT facts

U.S. DEPARTMENT OF ENERGY  
OFFICE OF FOSSIL ENERGY  
NATIONAL ENERGY TECHNOLOGY LABORATORY

Hydrogen and  
Clean Fuels from Coal

10/2007



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## EXPERIMENTAL DEMONSTRATION OF ADVANCED PALLADIUM MEMBRANE SEPARATORS FOR CENTRAL HIGH-PURITY HYDROGEN PRODUCTION

### Description

The United States has abundant reserves of coal that can be gasified and processed to provide the large amounts of hydrogen needed for the hydrogen economy. However, these gasification processes produce various contaminants that must be removed to obtain a stream of pure hydrogen. Past research has shown that palladium (Pd) alloys are promising candidates for the fabrication of robust membranes to separate hydrogen from coal gasification gases (syngas) or methane and associated contaminants. More specifically, trimetallic alloys of Pd, copper (Cu), and other metals have shown great potential in this area. The project team of United Technologies Research Center, Power & Energy, Inc., and Metal Hydride Inc., will confirm the stability and resistance of Pd Cu trimetallic alloys to carbon and carbide formation and resistance to sulfur, halides, and ammonia. They will develop a sulfur, halide, and ammonia resistant alloy membrane for hydrogen separation. The project will also provide a techno-economic evaluation of the use of Pd Cu trimetallic alloy hydrogen separators for central hydrogen production from coal, including an analysis of the optimal system configurations to use with the hydrogen separators. In addition, the project will design the engineering path to construct cost-effective separators for operation at high pressures.

### Primary Project Goals

- Confirm stability and resistance of Pd Cu trimetallic alloys to carbon and carbide formation, sulfur, halides, and ammonia
- Develop a sulfur, halide, and ammonia resistant Pd Cu trimetallic alloy membrane with a projected hydrogen permeance of  $25 \text{ m}^3\text{m}^{-2}\text{atm}^{-1}\text{h}^{-1}$  at  $400^\circ\text{C}$  and capable of operating at pressures of 12.1 MPa (~120 atm, 1750 psia)
- Complete advanced membrane property simulations by atomistic and thermodynamic modeling calculations
- Complete design and construction of six membrane separators using sulfur resistant palladium alloys and six membrane separators using proprietary Pd Cu<sup>TM</sup> alloys



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- Construct and experimentally validate the performance of each of the six Pd Cu alloy membrane hydrogen separators at feed pressures of 2 MPa (290 psia) in the presence of H<sub>2</sub>S, NH<sub>3</sub>, and HCl at a hydrogen production rate of 0.5 kg/day (10.6 L/min)
- Select and operate the optimal candidate separator for a minimum of 2,000 hours of continuous operation
- Complete hydrogen solubility tests using various alloys for six-to-twelve separators and predict hydrogen permeability performance
- Prepare a techno-economic evaluation on the use of Pd Cu trimetallic alloy hydrogen separators for central hydrogen production from coal gasifier fuel gas. Analyze optimum system configurations to use with these separators
- Define an engineering path to construct cost-effective separators for operation at pressures of 12.1 MPa (~120 atm)

## Accomplishments

None at present – New project initiated in FY-2007.

## Benefits

Trimetallic Pd Cu alloy membranes have been shown to exhibit high hydrogen selectivity and appear to have significant advantages over ceramic and polymer membranes in terms of manufacturability, lifetime (durability), ease of sealing, higher operating temperatures, and selectivity for hydrogen. The use of atomistic and thermodynamic modeling reduces costs for actual experimental tests by identifying optimal candidate alloy combinations for evaluation. The modeling effort provides quick evaluations on the performance of sulfur tolerant Pd-Cu bimetallic and trimetallic alloys.