Vehicle Technologies Office

Propulsion Materials Technologies

Jerry Gibbs
### Materials Technologies

**Values are FY15 enacted**

<table>
<thead>
<tr>
<th>Category</th>
<th>Lightweight</th>
<th>Propulsion</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY13 Enacted</td>
<td>$27.5 M</td>
<td>$11.9 M</td>
</tr>
<tr>
<td>FY14 Enacted</td>
<td>$28.0 M</td>
<td>$8.9 M</td>
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<tr>
<td>FY15 Enacted</td>
<td>$28.5 M</td>
<td>$7.1 M</td>
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#### Lightweight Materials
- **$28.5 M**
  - Properties and Manufacturing
  - Multi-Material Enabling
  - Modeling & Computational Mat. Sci.

#### Propulsion Materials
- **$7.1 M**
  - Engine Materials, Cast Al & Fe High Temp Alloys
  - Exhaust Sys. Materials, Low T Catalysts
  - Integrated Computational Materials Engineering
Propulsion Materials

• Targets powertrain materials requirements for future automotive and heavy-duty applications: engine, transmission, exhaust components, and targeted materials for electric powertrains. As the weight of the vehicle structure is reduced the percentage of the total vehicle weight in the powertrain is increasing.

• Addresses materials for high efficiency Internal Combustion Engines, powertrain materials interactions with new fuel compositions.

• Most (85%) Propulsion Materials projects utilize Integrated Computational Materials Engineering (ICME) to set performance targets and accelerate results in materials discovery, materials formulation, and materials processing techniques.

• Identifies gaps in existing ICME tools and develops new topics to expand the use of computational methods in materials development and materials engineering.
### Workshop Propulsion Materials R&D Gaps and Targets

<table>
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<tr>
<th>Metric</th>
<th>2013</th>
<th>2050</th>
<th>Material Gaps</th>
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</table>
| Powertrain Weight Reduction (ICE/HEV)       | Baseline - LDV  
Baseline – HDV | 40% lighter- LDV  
20% lighter- HDV   | Structure and Volumetric Efficiency (block, head, transmission; AL ,CF) |
|                                              |                                           |                                           |                                                                               |
|                                              |                                           |                                           |                                                                               |
| Power density                               | LDVs -2.7L 196 HP (73.4 HP/L)             | LD 1.3L 196 HP (150 HP/L)  
LW-LD 0.7L 98 HP | Structure and rotating components (crankshaft, pistons, connecting rods, gears; Steels + ) |
|                                              | HD15L 475HP (32 HP/L)                     | HD 9L 475HP (53 HP/L)                    |                                                                               |
|                                              |                                           |                                           |                                                                               |
| Energy Recovery                              | LDV <5% Turbocharged                      | LDV ~50% Turbo/ TEs/ Turbo-compounding   | Turbochargers, Superchargers, Turbo-compounding, Rankine Cycle components, seals, fluid interactions |
|                                              | HD ~99% Turbocharged                      | HD~ 99% Turbo/TEs/ Rankine Cycle/Turbo-compounding |                                                                               |
| Exhaust Temperatures (Exhaust Valve to Turbo Inlet) | LDV - 800 °C  
HDV - 700 °C | 1000 °C - LDV  
900 °C - HDV | Valves (super alloys & Ceramics) E Manifolds, Turbochargers |
| Cylinder Peak Pressures                      | LDV ~ 50 bar  
HDV  190 bar | >103 bar - LDV gasoline  
>150 bar ATP-DI gasoline  
>260 bar – HDV | Structure and rotating components , gaskets, valves, friction |
| Engine Thermal Efficiency                    | LDV 30% e  
HDV 42% e | LDV 45% e, Stretch 55+% e  
HDV 55% e, Stretch 60% e | Control Heat Losses (Pistons, Cylinder wall, Cylinder head, exhaust manifold) |
### Propulsion Materials Program

**Light- and Heavy-Duty Roadmaps, US Drive Low T Catalyst Workshop Report**

#### Engine Materials

- **Improve Engine Efficiency**
  - Improved Materials
  - Strength
  - Durability
  - Operating T
  - Manufacturability
  - Lower Cost

#### Exhaust System Materials

- **Low Cost High Temp Alloys for Exhaust Manifolds, Turbocharger Housings and Turbines**
- **Low Temp Catalyst Materials and ceramic substrates**

#### Integrated Computational Materials Engineering

- **New materials and processes using multi-scale modeling**
  - Modeling to create tailored materials
  - Predict behavior
  - Optimizing complex processes

#### Demonstration, Validation, and Analysis
Targets the Advanced Combustion Engine team stretch goals, 50%+ efficiency for heavy-duty and automotive engines

- **Lightweight Cast alloys for automotive engines and transmissions**: GM; Ford; ORNL/Chrysler: Lightweight high strength aluminum alloy development to replace A356 or A319 and enable higher operating temperatures and higher efficiency combustion regimes.

- **High performance Cast Ferrous Alloys for Heavy-duty Applications**: Caterpillar: High strength, low cost cast alloy development to provide performance superior to Compacted Graphite Iron, easily cast and machined, and at a cost similar to cast iron, enabling engines with higher peak cylinder pressures and increased efficiency.

- **High performance Cast Steels for Crankshafts**: Caterpillar/GM: High performance low cost cast steel providing performance similar to high cost forged steel units, enabling a low cost pathway to increased engine efficiency in automotive and heavy duty applications.
The Propulsion Materials’ Cast alloy development program for engine applications combines first principals computational materials design, advanced characterization, and experimental validation resulting in new alloys and expanded ICME capabilities.
Propulsion Materials– Exhaust System Materials, Low T Catalysts

Materials Technologies $36.9 M

- Propulsion Materials $8.9 M
  - Engine Materials, Cast Al & Fe High Temp Alloys
  - Exhaust Sys. Materials, Low T Catalysts
  - Integrated Computational Materials Engineering
  - Materials for Hybrid and Electric Drive Systems

- Fundamental Catalyst Materials
  - **ORNL**: Evaluation of catalyst microstructures and

- Exhaust Aftertreatment Components
  - **ORNL/Ford**: Impacts of biofuels on component life and development of mitigation strategies
  - **ORNL**: Durability of diesel particulate filters

- Low Temperature Catalyst
  Competitive awards made FY-2014
  - **Ford/ORNL** - Automotive
  - **Chrysler (FCA)/PNNL** - Automotive
  - **Cummins/PNNL** – Heavy-Duty Trucks
The Propulsion Materials’ Low Temperature Catalyst development effort is guided by the US CAR advanced aftertreatment workshop report and all materials development and validation activities reside in the areas outlined in red bridging materials fundamentals and applied R&D.
Integrated Computational Materials Engineering

- **ORNL**: Exploratory methods based on First Principals Calculations, Density Functional Theory, and Calculated Density of States to identify new materials compositions with tailored properties:
  - Thermoelectric Materials, 3 new compositions have been validated;
  - Non-rare earth magnetic materials, 2 new compositions have been validated;
  - Low Temperature Catalyst materials, 1 new low temperature catalyst have been validated for Oxides of Nitrogen
- Each Propulsion Materials FOA project includes a multi-scale ICME application, validation, and gap analysis component (two were included in the President's Materials Genome announcement).
Materials Target Setting

Advanced Combustion Models

Temperature and pressure Boundary conditions

Efficiency improvement potential

Finite Element Baseline Design Constraints

Prioritized Components and Material Property Targets

Identify and prioritize the material improvements needed to enable high efficiency combustion systems, and quantify the benefits.
Propulsion Materials— Materials for Hybrid and Electric Drive Systems

- Projects very limited in scope to address specific gaps in material properties, materials processing, or material joining
  - **ORNL**: Enabling Materials for High Temperature Electronics: Organic materials not 200°C-capable
  - **ORNL**: Enabling Materials for High Temperature Electronics: Solders not 200°C-capable
  - **PNNL**: Novel Manufacturing Technologies for High Power Induction and Permanent Magnet Electric Motors
- Goal to rapidly transition results to the APEEM team

New non-rare earth magnetic materials are predicted within the ICME activity and validated by the APEEM team
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