Overview of the DOE Advanced Combustion Engine R&D Program

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Outline

- State of technology today for ICE
- Overview of the Advanced Combustion Engine R&D Program
- Combustion and Emission Control Subprogram
  - Engine Combustion Research
    - Low Temperature Combustion
    - Predictive Simulation for ICE Design
  - Emission Control R&D
  - High Efficiency Engine Technologies
- Solid State Energy Conversion Subprogram
- Summary
Opportunity for Increased ICE Efficiency

*Increasing the efficiency of internal combustion engines (ICEs) is one of the most promising and cost-effective approaches to improving the fuel economy of the U.S. vehicle fleet in the near- to mid-term.*

“The performance, low cost, and fuel flexibility of ICEs makes it likely that they will continue to dominate the vehicle fleet for at least the next several decades. ICE improvements can also be applied to both hybrid electric vehicles (HEVs) and vehicles that use alternative hydrocarbon fuels.” DOE QTR 2011

“...ICEs ... are going to be the dominant automotive technology for decades, whether in conventional vehicles, hybrid vehicles, PHEVs, biofueled or natural gas vehicles. ...better understanding of the combustion process and emissions production can help to overcome a major barrier to more advanced ICEs, this work is important to the country. ...” NRC Report 2013

EIA AEO 2014 reference case scenario - even by 2040, **over 99% of vehicles sold will have ICEs.**

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1. Quadrennial Technology Review, DOE 2011
Increase in internal combustion engine performance has been largely responsible for significant fuel economy increases (in spite of increases in vehicle size and weight).

**Progress In Heavy-Duty Diesel Engine Efficiency and Emissions**

**Historical progress in heavy-duty engine efficiency and the challenge of simultaneous emissions reduction, illustrate positive impact from DOE R&D support.**

- DOE R&D improved thermal efficiency of over-the-road heavy-duty diesel engines by over 4.5%.
- Benefits from heavy-duty vehicles alone (1995 – 2007) represent an over 70:1 return on investment (ROI) of government funds for heavy-duty combustion engine R&D - total savings of over $70B.

**Historical Trend in Emissions from New Diesel Engines**

“We have been working with DOE on clean engine technology for the past 20 years. In fact, many of the technologies used in our engines today were developed in partnership with the DOE, our national labs, universities and other research institutions.” – Tim Solso, Cummins Chairman and CEO, June 2010.

Advanced Combustion Engine R&D

**Strategic Goal:** Reduce petroleum dependence by removing critical technical barriers to mass commercialization of high-efficiency, emissions-compliant internal combustion engine (ICE) powertrains in passenger and commercial vehicles

**Primary Directions**
- Improve ICE efficiency through advanced combustion strategies
- Develop aftertreatment technologies
- Explore waste energy recovery with mechanical and advanced thermoelectric devices

**Performance Targets**

<table>
<thead>
<tr>
<th></th>
<th>Light-Duty</th>
<th>Heavy-Duty</th>
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<tr>
<td></td>
<td>2015</td>
<td>2020</td>
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<tr>
<td>Engine brake thermal efficiency</td>
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<td>--</td>
</tr>
<tr>
<td>Fuel economy improvement</td>
<td>25 – 40%</td>
<td>35 – 50%</td>
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<tr>
<td>NOx &amp; PM emissions</td>
<td>Tier 2, Bin 2</td>
<td>Tier 3/LEV III</td>
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*compared to 2009 model year baseline
## Advanced Combustion Engine R&D Program:
**Budget by Subprogram**

<table>
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<tr>
<th>Major Activities</th>
<th>FY 2013 Current</th>
<th>FY 2014 Enacted</th>
<th>FY 2015 Request</th>
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<tr>
<td>Advanced Combustion Engine R&amp;D</td>
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<td>$49,970K</td>
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<td>Combustion and Emission Control</td>
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<td>Solid State Energy Conversion</td>
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** FY 2013 full year CR inclusive of SBIR/STTR.
*** FY 2014 budget request inclusive of SBIR/STTR.
Advanced Combustion Engine R&D

Strategic Goal: Remove critical technical barriers to mass commercialization of high-efficiency, emissions-compliant internal combustion engine (ICE) powertrains in passenger and commercial vehicles

Advanced Combustion Engines Program

Combustion and Emission Control

Combustion R&D

Emission Control R&D

High Efficiency Engine Technologies

Solid State Energy Conversion

Sandia National Laboratories

Engine Combustion Research.

Data from multiple advanced laser diagnostics have substantially improved understanding of engine combustion and emissions formation.

Fuel concentration

Soot (red) and OH (green)

PNNL DPF Model

21% O₂ \( \phi_d(H) = 2.7 \)

9% O₂ \( \phi_d(H) = 2.9 \)

BMW X6
Overall R&D Approach

**Advanced Combustion Engine R&D**

**Fundamental Research**
- SNL – Advanced Combustion Strategies (LTC, lean-burn gasoline, advanced Diesel)
- LLNL – Chemical kinetics models (Combustion, fuels and emissions)
- LANL – CFD modeling of combustion
- ANL – X-ray fuel spray characterization
- PNNL – Catalyst Characterization (NOx and PM Control)
- Universities – Complementary research

**Applied Research**
- Fundamental to Applied Bridging R&D
  - ORNL – Experiments and simulation of engines and emission control systems (bench-scale to fully integrated systems)
  - ANL – fuel injector design, LTC engine experiments

**Technology Maturation & Deployment**
- Competitively Awarded Cost-shared Industry R&D
  - Automotive and engine companies,– engine systems
  - Suppliers – enabling technologies (sensors, ignition, VVA, WHR)

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**Improved Understanding**

**Advanced Concepts**

**R&D Needs**

**Technical Barriers**

**Commercial Product**
- Explore low-temperature combustion strategies to achieve higher engine efficiencies with near-zero emissions of NOx and PM.
- Develop greater understanding of engine combustion and in-cylinder emissions formation processes.
- Develop science-based, truly predictive simulation tools for engine design.
Goal: To develop the knowledge base for low-temperature combustion (LTC) strategies and carry research results to products.

- Science-base for advanced combustion strategies
- Computational tools for combustion system design and optimization
- Identify potential pathways for efficiency improvement and emission compliance

Close collaboration with industry through the Advanced Engine Combustion MOU led by Sandia National Labs *carries research to products.*

Cross cuts light-duty and heavy-duty engine R&D

University research* integrated with MOU

*Funded under the NSF/DOE Partnership on Advanced Combustion Engines
Close coupled modeling and experiments
- Advanced diagnostics including optical, laser, x-ray, and neutron based techniques
- Multi-dimensional computational models and combustion simulators
- Fuel kinetics
- Multi- and single-cylinder engines

Close collaboration between industry, national labs and universities

Cross-cuts light- and heavy-duty engine R&D

Leading to engine CFD modeling tools widely used in industry
Combustion Research Directions and Challenges

Combustion Strategies Enabling Improved Efficiency and Very-Low Emissions

- **Low-Temperature Combustion (LTC):**
  - Premixed-Charge Compression-Ignition (PCCI) (PPCI, PCI, MK, …) – “mixed enough”
  - Homogeneous-Charge Compression-Ignition (HCCI) – “heterogeneous enough”
  - Reactivity Controlled Compression Ignition (RCCI) – “dual fuel” combustion

- **Dilute Gasoline Combustion:** Fuel-air mixing, ignition and flame propagation in stratified mixtures, stochastic misfire and knock challenges, fuels, emissions…

- **Clean Diesel Combustion:** EGR, high-pressure and multi-pulse injection, lifted-flame combustion, post injections for in-cylinder and aftertreatment emission control…

- **LTC Challenges:**
  - Combustion phasing
  - Load range
  - Heat release rate
  - Transient control
  - HC and CO emissions
  - Fuel characteristics
Diesel and HCCI Combustion

Conventional Diesel Combustion
(movie of hot, glowing soot)

- fuel injector (center) sprays 8 jets of liquid fuel into combustion chamber
- compression-heating ignites fuel
- soot forms in fuel-rich jets, and glows red/orange/yellow
- some soot escapes combustion ⇒ soot emissions
- high-temperature combustion = high NOx
- high efficiency

Homogeneous Charge Compression Ignition
(movie of combustion chemiluminescence)

- fuel is vaporized and premixed with air prior to compression
- compression-heating ignites fuel
- mixtures are fuel-lean so no soot forms, but combustion reactions emit light (blue)
- no soot emissions
- low-temperature combustion = low NOx
- high efficiency
Workshops to Identify R&D Needs

Combustion Engine Efficiency Colloquium, USCAR Detroit, MI, March 3 – 4, 2010

Findings

- Achievable peak efficiencies > 60%, “affordable” engines may be lower.
- Possible 2X improvement in fuel efficiency for LD vehicles.

Highest Priority Industry Barriers For Advanced Engines (BES/VTO PreSICE workshop focus)

- Effect of stochastic nature of in-cylinder flow on engine combustion, performance and emissions
- Spray modeling and experimentation in dense spray and nozzle internal flow regions, including physics like cavitation and flash boiling.

Workshop on Predictive Simulation of ICE (PreSICE), March 3, 2011
Product Development Must Be Accelerated To Meet Energy Goals

Achievable efficiency improvements:
Auto: 50%, Truck: 30%

With predictive modeling:

R&D

Business as usual:

Product Development Cycles

Full Market Transition

Conversion to CO₂ Neutral Infrastructure

2000 2010 2020 2030 2040 2050
World-class HPC expertise and resources applied to address engineering challenges (technology barriers) once thought unsolvable

Example ORNL projects in collaboration with industry

- **Understanding stochastic and deterministic processes driving cyclic variability in highly dilute SI engines and their impacts on efficiency**
  - Major challenge is scaling serial problem (cycle-to-cycle variations) to parallel computation architecture

- **Understanding and optimizing fuel injector design for improved efficiency and reduced emissions**
  - Computational framework for coupling models of internal injector flow and cavitation with in-cylinder spray and combustion

Development and validation of models to enable simulation of stochastic processes

- Sub-grid scale models for unresolved processes
- Reduced chemical kinetic mechanisms
- New theoretical frameworks / efficient numerical approaches

Complex in-cylinder flow during intake stroke in diesel engine

General Motors Research
High Performance Computing Could Accelerate Engine Design and Optimization

Basic Science

DOE Office of Science
Fundamental expertise in combustion instability mechanisms and leadership in high performance computing including the world’s fastest supercomputer.

Applied R&D

DOE/EERE/VTO
Accelerating high pressure fuel injector design optimization and providing new insights into combustion instability phenomena.

Manufacturing/Commercialization

GM/Ford/GE
Research in close collaboration with automobile and engine manufacturers will directly impact the development of the next generation of high efficiency engines.

TITAN Use Awards
- ALCC 32.5M hrs
- OLCF 17M hrs

Making use of unique world class resources to address real-world challenges.
Cyclic Variability with Large Eddy Simulations

Project Impact
• High-fidelity Large Eddy Simulations (LES) can capture flow structures which lower fidelity (RANS) approaches cannot predict
• LES can predict cycle-to-cycle variations during each injection event. Further research to predict engine misfire!

Experimental data: Sandia National Laboratory

Computational Details
• High-temporal and spatial resolutions results in less sub-grid scale modeling with the LES
• Each cycle: 1 month on 256 cores; need at least 8-10 cycles
• Simulations performed at Fusion cluster at Argonne together with Cummins Engine Company and Convergent Science Inc.
Multi-hole Nozzle Two-phase Flow Simulations

Project Impact
• Plume-to-plume variations in Multi-hole nozzles can now be captured
• Influence of needle transients on fuel spray development can now be predicted!

Computational Details
• High-temporal and spatial resolutions resulting in grid-convergent solutions
• Each Simulation: 1 month on 64 cores; Need 20+ simulations

Time = 0.000100

Production GM multi-hole diesel injector simulation at Argonne
Fuel Economy Optimization with High-Fidelity Simulations

Project Impact

- Specific fuel consumption was **optimized using genetic algorithm** based tools and CONVERGE CFD code for **Chrysler LLC**.
- Predicted optimized speed-load conditions corroborated very well with experimental measurements on a Chrysler Dual-fuel combustion engine at Argonne.
- The **optimized conditions also showed considerably lower emissions** compared to the baseline.

Computational Needs

- 400 engine simulations performed to achieve optimized fuel economy and emissions.
- Each simulation generation takes about a week on 24 cores.
Intra-nozzle Fuel Injector Processes Being Studied Using Neutron Radiography

- Neutrons easily penetrate metal injectors with low interactions and offer opportunity to study critical internal fuel flow dynamics (e.g. cavitation)
- Neutrons readily diffracted/adsorbed by hydrogen containing hydrocarbons, like fuel
  - Complements X-ray and laser-based optical approaches being done in other DOE projects
- Demonstrated tomographic capability; moving towards dynamic image operation
  - 20 micro-second frames and 1 ms injections

Bright areas are fuel
Numerical tools and High Performance Computing (HPC) enable more predictive CFD of Advanced Combustion Regimes (LLNL)

- Prediction of kinetically controlled combustion and emissions requires simulations with highly detailed chemistry
  - Enabled by multi-zone and adaptive preconditioning work at LLNL
  - HCCI simulations of gasoline surrogate (~1400 species) can now be run in less than 24 hours.

- HPC provides opportunity to examine experimental and modeling uncertainties systematically
  - Reduces the necessary “tuning” of models to experiments
  - Results in more predictive engine models

- Incorporating graphics processing unit (GPU) algorithms into CFD codes ensures continued improvement in modeling capability as computing platforms move towards massively parallel architectures.
• Develop more efficient approaches for reducing NOx, and oxidizing PM, HC and CO in low temperature exhaust (150°C)
• Reduce energy penalty and cost of emission control systems
CLEERS Facilitates Technical Exchange Across Universities, National Labs, and Industry

- Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) enables technical cross-talk on emission control technology via web meetings, data and model sharing, workshops, and the website www.cleers.org
- More than 100 representatives from industry, national labs, and universities attended the recent workshop in Dearborn, MI

Global model accurately predicts NH₃ formation inside LNT catalyst during regeneration

BASF
Bosch
Caterpillar Inc.
Chalmers University
Cummins Inc.
Delphi
Detroit Diesel Corporation
Eaton Corporation
Ford Motor Company
Gamma Technologies
General Motors*
Hilite
John Deere
Johnson Matthey
Mack Powertrain
MECA
Michigan Technological University
Navistar
Northwestern University
Oak Ridge National Laboratory*
Pacific Northwest
National Laboratory*
Sud-Chemie
Tenneco Inc.
Umicore
University of Michigan
University of Wisconsin
Sandia National Laboratories
Sud-Chemie
Tenneco Inc.
Umicore
University of Wisconsin
*Organizers
EERE VTO Catalysis Research for Vehicles Spans from Nanoscale to Full Scale

**Research Areas**

- **Surface Chemistry**
  Defining surface moieties and intermediates with DRIFTS and other tools

- **PGM Characterization**
  Defining Platinum Group Metal (PGM) roles and understanding sintering processes

- **Poison Effects**
  Understanding effect of fuel- and oil-borne poisons/fouling agents on aging processes

- **Reaction Mechanisms**
  Characterizing reaction processes and measuring kinetics

- **Characterizing Formulation-Specific Chemistry**
  Understanding role of components of complex heterogeneous catalyst formulation

- **Performance and Selectivity**
  Measuring formulation affect on performance and selectivity (including differentiating regulated vs. unregulated products)

- **Controlling Unique Advanced Combustion Emissions**
  Studying combination of advanced catalysts with advanced combustion to achieve overall gains in fuel economy and cost-effective emission compliance

- **Minimizing Fuel Penalty during Active Regeneration**
  On-engine studies to minimize fuel use and optimize emission control

- **Characterizing Combustion-Specific PM and MSATs**
  Defining morphology, size distribution, and chemical composition of Particulate Matter (PM) and Mobile Source Air Toxics (MSATs)

- **Particulate Filter-Based Control of PM**
  Studying oxidation kinetics, thermal issues, and fuel penalty for particulate filters

**Industry Benefits**

- Understanding Catalyst Fundamentals
- Predicting Degradation and Defining Mitigation Strategies
- Developing and Validating Models for Product Design, Controls, and OBD Optimization
- Achieving Cost-Effective Emissions Compliance while Maximizing Fuel Efficiency
U.S.DRIVE workshop conducted to develop a roadmap to address “The 150°C Challenge” related to future automotive emission control in highly efficient engines with low exhaust heat energy and new gas chemistries.
Advanced combustion techniques offer higher fuel efficiency but emission control challenges exist.

LTC gives lower exhaust temperatures and higher HC and CO emissions relative to conventional diesel combustion (CDC).

Catalysts with improved low temperature oxidation performance are being developed and studied to enable commercial viability.
Low Temperature Catalysis Research Addresses New Challenges of Advanced Engines

Basic Science
DOE Office of Science

New materials showing excellent low temperature performance and durability

Applied R&D
DOE/EEERE/VTO

Materials being evaluated under real-world conditions to understand potential with high efficiency combustion strategies

Manufacturing/Commercialization
Industry

Supporting automobile and truck manufacturers in the development and execution of a path forward to address this critical enabler for high efficiency engines

Transitioning catalyst material breakthroughs to overcome critical barriers to high efficiency transportation
Low Temperature Emission Control Improvements Enabling Commercialization of Advanced Combustion

Catalyst invented in Basic Energy Sciences (BES) program leading to new discoveries in VTO program that may enable low cost emission control for advanced engines

\[ \text{CuO}_x\text{-CoO}_y\text{-CeO}_2 \text{ (CCC)} \]

*CuO\textsubscript{x}-CoO\textsubscript{y}-CeO\textsubscript{2} (CCC) catalyst developed in BES program contains no costly Platinum Group Metals*

Unlike Pd-based catalysts, VTO studies show CCC’s CO oxidation not inhibited by HCs (a unique finding)

Low-cost catalyst may address higher CO and HC emissions and lower exhaust temperatures of LTC

More Fuel Efficient* Low Temperature Combustion (LTC) gives higher CO & HCs*

And lower exhaust temperatures*

*vs. Conventional Diesel Combustion
$12M over 3 years, equally shared by each agency - *Jointly funded by the DOE Vehicle Technologies Office of the Office of Energy Efficiency and Renewable Energy and the National Science Foundation Division of Chemical, Bioengineering, Environmental, and Transport Systems, Directorate of Engineering*

**Combustion Research**
- University of California, Berkeley - $1.65M
- Michigan State University - $1.30M
- Michigan Technological University - $0.65M
- University of New Hampshire - $0.60M
- The Pennsylvania State University - $0.60M
- University of Connecticut - $0.80M
- Stanford University - $1.2M
- Clemson University - $1.0M
- Yale University - $0.60M

**Emission Control Research**
- University of Kentucky - $0.90M
- University of Houston - $1.20M
- Purdue University - $1.50M
• Develop and demonstrate system level technologies to improve vehicle fuel economy through combination of combustion strategies, emission control, fuel injection, air handling, waste heat recovery, and control systems.
SuperTruck Initiative

- **June 2009**: Solicitation ... develop and demonstrate a 50% improvement in overall freight efficiency on a heavy-duty Class 8 tractor-trailer, measured in ton-miles per gallon; achieve 50% engine thermal efficiency at 65 mph and show a pathway to 55% engine efficiency.
  - Both engine and vehicle system technologies included
  - Vehicle target for freight efficiency (ton-miles per gallon) improvement based on 65,000 pound GVW
  - 40% of the total improvement is required from engine technologies (50% thermal efficiency) and the remainder from vehicle system technologies.

Daimler Trucks North America \( \text{VOLVO} \) \( \text{NAVISTAR} \)
SuperTruck - Develop and Demonstrate System Level Technologies to Improve Long Haul Truck Freight Efficiency

- Heavy-Duty Engine for Class 8 Trucks
  - 20% improvement in engine brake thermal efficiency (50% BTE)
  - Modeling and analysis for pathway to 55% brake thermal efficiency

Status of 50% engine efficiency:
- Cummins and Daimler have demonstrated over 50% brake thermal efficiency for SuperTruck laboratory engine
- Navistar and Volvo have demonstrated over 48% engine efficiency and are on track to meet goal.
Advanced Technology Powertrain for Light-Duty (ATP-LD) Vehicles

Develop and Demonstrate System Level Technologies to Improve Vehicle Fuel Economy

- **Light-Duty Vehicles**
  - 25% fuel economy improvement for gasoline engines over baseline*
  - 40% fuel economy improvement for diesel engines over baseline*

- **Status**
  - GM and Chrysler achieved 25% fuel economy improvement.
  - Ford and Bosch are on track to achieve 25% fuel economy improvement.
  - Cummins is on track to achieve 40% fuel economy improvement.
  - Delphi demonstrated potential for 50 percent increase in light-duty vehicle fuel economy

*Baseline is state-of-the-art port-fuel injected 2009 gasoline engine

- Simulations predict very good fuel economy on U.S. cycles with LTC engine
Enabling Technologies for Engine and Powertrain System

- General Motors LLC completed dynamometer testing and established fuel efficiency at 11 speed-load test points for a production turbocharged engine modified with 11:1 compression ratio, high energy (DCO™) ignition system, and dedicated low pressure loop (LPL) EGR system.

- Eaton Corporation developed a three stage Roots expander for testing in a heavy duty engine organic Rankine cycle (ORC) waste heat recovery system.

- MAHLE Powertrain LLC validated with pre-chamber simulation, multiple distributed ignition sites with turbulent jet injection for the next-generation ultra lean burn engines.

- Filter Sensing Technologies (FST) Inc. demonstrated on-vehicle, a particulate matter (PM) radio frequency sensor and electronic control system that reduces the cost and fuel penalty of diesel particulate filters (DPFs).
Enabling Technologies for Engine and Powertrain System

- Robert Bosch LLC developed an intake air oxygen (IAO2) sensor that directly and accurately measures the oxygen concentration in the intake manifold for accurate and robust EGR control for future engine concepts.

- LANL completed engine dynamometer testing of its robust Nitrogen Oxide/Ammonia Sensors providing quantitative correlation of NOx response to FTIR and HC response to FID THC content during start up and EGR on/off operations.

- Envera LLC completed the design of a variable compression ratio (VCR) engine incorporating variable valve actuation (VVA) and new supercharging technology.
Solid State Energy Conversion

• Develop and demonstrate advanced thermoelectric systems to improve vehicle fuel economy by converting energy in the engine exhaust directly to electricity.

Competitively selected cost-shared 2\textsuperscript{nd} Generation TEG projects:

- GenTherm
- General Motors
- GMZ Energy

Develop commercially viable advanced TEGs, improved technology for manufacturing TE devices, and assess feasibility and cost reduction for production volumes of 100,000 units per year.
Summary

- Light-duty engine performance improvements have been largely responsible for passenger vehicle fuel economy increases (in spite of vehicle weight, horsepower and size increases).

- Continued improvement in heavy-duty engine efficiency and emissions has been responsible for significant fuel savings in commercial vehicles.

- EERE Advanced Combustion Engine R&D, in collaboration with industry and academia, using unique Federal laboratory expertise and facilities, significantly contributes to dramatic increases in engine efficiency and performance, improvements in vehicle fuel economy, and reduction in emissions and transportation energy use.

- There is still significant potential for further efficiency (fuel economy) improvements using Low-Temperature Combustion and engine optimization:
  - Potential for 50% FE improvement for light-duty vehicles
  - Over 30% FE improvement for heavy-duty vehicles

- Combustion and emission control system modeling and simulation has reduced product development time and improved engine efficiency.
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