A Workshop to Identify Research Needs and Impacts in Predictive Simulation for Internal Combustion Engines (PreSICE)

Sponsored by the Office of Basic Energy Sciences, Office of Science and the Vehicle Technologies Program, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy

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This report is available on the web at:
http://www.sc.doe.gov/bes/reports/files/PRESICE_rpt.pdf

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Executive Summary

Executive Summary

The U.S. has reached a pivotal moment when pressures of energy security, climate change, and economic competitiveness converge. Oil prices remain volatile and have exceeded $100 per barrel twice in five years. At these prices, the U.S. spends $1 billion per day on imported oil to meet our energy demands. Because the transportation sector accounts for two-thirds of our petroleum use, energy security is deeply entangled with our transportation needs. At the same time, transportation produces one-quarter of the nation's carbon dioxide output. Increasing the efficiency of internal combustion engines is a technologically proven and cost-effective approach to dramatically improving the fuel economy of the nation's fleet of vehicles in the near- to mid-term, with the corresponding benefits of reducing our dependence on foreign oil and reducing carbon emissions. Because of their relatively low cost, high performance, and ability to utilize renewable fuels, internal combustion engines—including those in hybrid vehicles—will continue to be critical to our transportation infrastructure for decades. Achievable advances in engine technology can improve the fuel economy of automobiles by over 50% and trucks by over 30%.

Achieving these goals will require the transportation sector to compress its product development cycle for cleaner, more efficient engine technologies by 50% while simultaneously exploring innovative design space. Concurrently, fuels will also be evolving, adding another layer of complexity and further highlighting the need for efficient product development cycles. Current design processes, using "build and test" prototype engineering, will not suffice. Current market penetration of new engine technologies is simply too slow—it must be dramatically accelerated.

These challenges present a unique opportunity to marshal U.S. leadership in science-based simulation to develop predictive computational design tools for use by the transportation industry. The use of predictive simulation tools for enhancing combustion engine performance will shrink engine development timescales, accelerate time to market, and reduce development costs, while ensuring the timely achievement of energy security and emissions targets and enhancing U.S. industrial competitiveness.

In 2007 Cummins achieved a milestone in engine design by bringing a diesel engine to market solely with computer modeling and analysis tools. The only testing was after the fact to confirm performance. Cummins achieved a reduction in development time and cost. As important, they realized a more robust design, improved fuel economy, and met all environmental and customer constraints. This important first step demonstrates the potential for computational engine design. But, the daunting complexity of engine combustion and the revolutionary increases in efficiency needed require the development of simulation codes and computation platforms far more advanced than those available today.

Based on these needs, a Workshop to Identify Research Needs and Impacts in Predictive Simulation for Internal Combustion Engines (PreSICE) convened over 60 U.S. leaders in the engine combustion field from industry, academia, and national laboratories to focus on two critical areas of advanced simulation, as identified by the U.S. automotive and engine industries. First, modern engines require precise control of the injection of a broad variety of fuels that is far more subtle than achievable to date and that can be obtained only through predictive modeling and simulation. Second, the simulation, understanding, and control of these stochastic in-cylinder combustion processes lie on the critical path to realizing more efficient engines with greater power density.

Fuel sprays set the initial conditions for combustion in essentially all future transportation engines; yet today designers primarily use empirical methods that limit the efficiency achievable. Three primary spray topics were identified as focus areas in the workshop:

1. The fuel delivery system, which includes fuel manifolds and internal injector flow,
2. The multi-phase fuel–air mixing in the combustion chamber of the engine, and
3. The heat transfer and fluid interactions with cylinder walls.

Current understanding and modeling capability of stochastic processes in engines remains limited and prevents designers from achieving significantly higher fuel economy. To improve this situation, the workshop participants identified three focus areas for stochastic processes:

1. Improve fundamental understanding that will help to establish and characterize the physical causes of stochastic events,
2. Develop physics-based simulation models that are accurate and sensitive enough to capture performance-limiting variability, and
3. Quantify and manage uncertainty in model parameters and boundary conditions.

Improved models and understanding in these areas will allow designers to develop engines with reduced design margins and that operate reliably in more efficient regimes.

All of these areas require improved basic understanding, high-fidelity model development, and rigorous model validation. These advances will greatly reduce the uncertainties in current models and improve understanding of sprays and fuel–air mixture preparation that limit the investigation and development of advanced combustion technologies.

The two strategic focus areas have distinctive characteristics but are inherently coupled. Coordinated activities in basic experiments, fundamental simulations, and engineering-level model development and validation can be used to successfully address all of the topics identified in the PreSICE workshop. The outcome will be:

1. New and deeper understanding of the relevant fundamental physical and chemical processes in advanced combustion technologies,
2. Implementation of this understanding into models and simulation tools appropriate for both exploration and design, and
3. Sufficient validation with uncertainty quantification to provide confidence in the simulation results.

These outcomes will provide the design tools for industry to reduce development time by up to 30% and improve engine efficiencies by 30% to 50%. The improved efficiencies applied to the national mix of transportation applications have the potential to save over 5 million barrels of oil per day, a current cost savings of $500 million per day.

Introduction

Introduction

The U.S. stands at a critical juncture where pressures of energy security, environmental concerns, and economic competitiveness converge. Political instabilities in other parts of the world serve as nearly constant reminders of the economic and national security risks of importing almost two-thirds of our petroleum. The transportation sector accounts for two-thirds of the nation's oil use and one-quarter of its greenhouse gas emissions. In 2008 the United States had some 300 million automobiles and light-duty trucks on the road that used approximately 130 billion gallons of gasoline per year and created an annual environmental burden of 1.2 billion metric tons of CO_2. Diesel engines in the U.S. are estimated to burn a further 50 billion gallons of fuel per year, so combustion of liquid fuels in the U.S. annually adds close to 1.5 billon metric tons of CO_2 into the environment. The transportation sector lies at the crossroads of our nation's energy and environmental security. Aggressive national goals for reducing petroleum use by 17% by 2020 and greenhouse gas emissions by 83% by 2050 will require major improvements in all aspects of our energy use. Meanwhile, the U.S. vehicle industry labors under tremendous pressure from international competitors and challenging economic conditions.

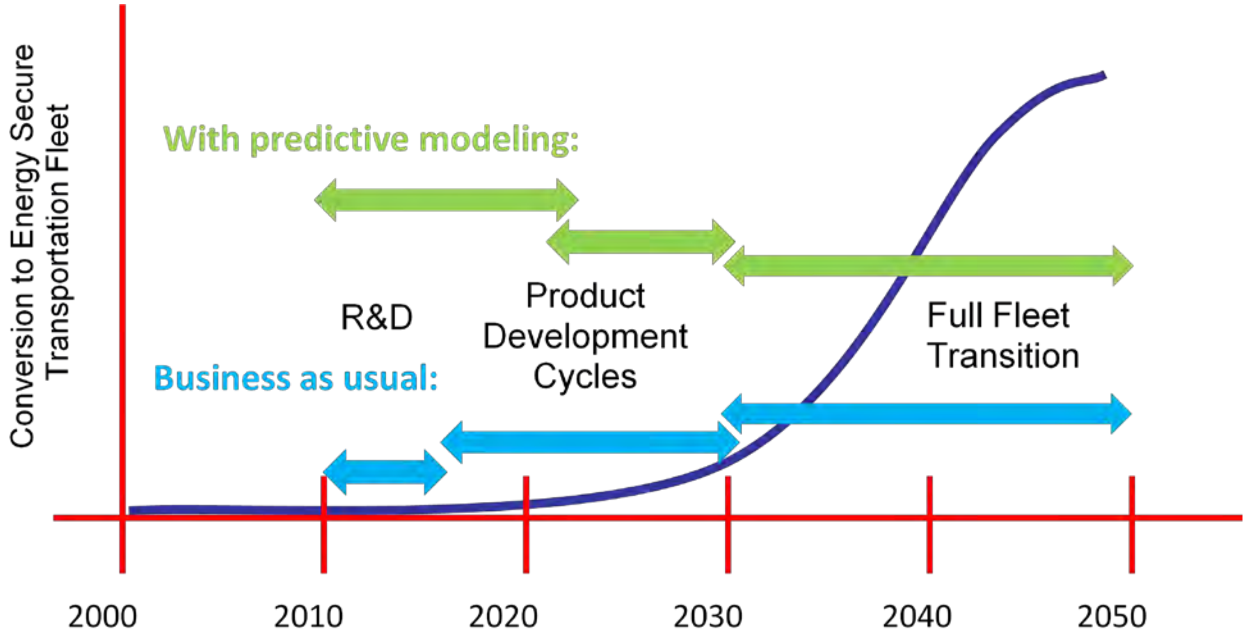

Figure 1. Realizing a 2050 vehicle fleet that reduces petroleum use by 83% requires investments in the next decade to meet the timeline. Current 20 year vehicle life requires that by 2030 all vehicles sold must embody the minimum technology to meet 2050 goals. *(Figure courtesy of PreSICE workshop)*

While the 2050 goals may at first appear to be distant in time with little need for urgent action, a closer look reveals a strong case for immediate and sustained action, as shown in Figure 1. To effect substantial change by 2050, the current 20-year vehicle fleet turnover time requires that, starting in 2030, all vehicles sold must embody the clean and efficient technologies required for 2050. A high-efficiency drive train must become as widespread as air bags are today—not an option, but rather a common feature on all vehicles. Current engine development cycles typically require three generations lasting five years each to move a new technology from the first commercial demonstration to being widely available throughout a product line. Such a 15 year process steps the timeline back to 2015 as the date when these new technologies would need to be commercially ready to meet 2050 goals, which leaves only a few years to undertake the foundational research and development. This brief period is widely believed to be unrealistically short to achieve the transformational technology improvements required for the 2050 vision.

Even independent of a 2050 goal, timely action to sustain the energy security and competitiveness of the U.S. transportation sector will require manufacturers to condense the product design and commercialization cycle for cleaner, more efficient engine technologies in order to provide more time for the required research and development. Other industries have demonstrated that applying predictive, computer-based simulation can shrink product development cycles by up to a factor of three while simultaneously producing better products more cheaply. The Council on Competitiveness has documented these successes in industries ranging from soap to tires to aircraft.[1] With the application of advanced predictive simulation, the U.S. transportation industry will be able to market competitive, clean, and efficient products in a timeframe that meets national needs.

A transportation fleet that consumes 83% less petroleum and produces 83% less carbon dioxide in 2050 is expected to require the implementation of three simultaneous and complementary strategies: enhanced efficiency of internal combustion engines, deployment of alternative fuels such as biofuels, and increasing levels of vehicle electrification ranging from current hybrids to plug-in hybrids and full electric vehicles. Increasing the efficiency of internal combustion engines is the most direct and cost-effective approach to improving the fuel economy of the nation’s fleet of vehicles in the near- to mid-term. Because of their relatively low cost, high performance, and ability to utilize renewable fuels such as ethanol, biodiesel, and second-generation biofuels, combustion engines will likely dominate the market for several decades. Advanced combustion technologies can provide substantial improvements in efficiency, up to 50% or more, as identified in a recent workshop report from Oak Ridge National Laboratory.[2] Using these advanced engines in hybrid electric vehicles (HEV) and plug-in HEVs (PHEV) will enable even greater fuel savings. Thus, while industry and the DOE continue to actively pursue alternative non-hydrocarbon methods of propulsion for transportation, improvements in engine efficiency both for petroleum-based fuels and alternative biofuels clearly can have a major payoff both in reducing petroleum consumption and emissions, and improving energy security within the United States—if they can rapidly enter the transportation market in sufficient numbers.

These challenges present a unique opportunity to marshal U.S. leadership in predictive modeling of engineered systems and in supercomputing to develop predictive computational design tools for use by the transportation industry. Using predictive simulation tools for enhancing combustion engine performance will shrink engine development timescales, accelerate time to

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[1] http://www.compete.org/publications/.

[2] See the “Summary Report on the Transportation Combustion Engine Efficiency Colloquium Held at USCAR, March 3 and 4, 2010,” ORNL, http://www.osti.gov/bridge/product.biblio.jsp?query_id=0&page=0&osti_id=993029&Row=0.

market, and reduce development costs, all while ensuring the timely achievement of energy security and emissions targets, and enhancing the competitiveness of U.S. engine manufacturers.

In 2007 Cummins achieved a milestone in engine design by bringing a diesel engine, the 2007 ISB 6.7 liter, to market solely with computer modeling and analysis tools. The only testing was after the fact to confirm performance. Cummins achieved a reduction in development time and cost (estimated to be about 10% for this first effort). As important, they realized a more robust design, improved mileage, and met all environmental and customer constraints. While an important milestone, the achievement was an incremental step in the use of computational modeling. In other industries such as tire manufacturing, acceleration of product design by a factor of three has been realized through implementing robust predictive design tools. The daunting complexity of engine combustion, up to a million times more complex than tires, requires the development and application of equally advanced simulation codes and computation platforms for combustion.

Developing such predictive tools is a significant scientific and technical challenge that lies beyond the capability of industry alone to achieve. The automotive and engine industries are intensely competitive on the international scale. These industries have neither the time nor the resources to invest in an R&D program of this extent. Pre-competitive investment in partnerships between academia, national laboratories, and industry are both appropriate and required. There is ample historical precedent for such investment in combustion simulation. The two foundational tools for current computational engine design—Kiva, a fluid dynamics tool, and Chemkin, a chemistry tool—grew initially out of research efforts at Los Alamos Laboratory, Sandia National Laboratories, and their academic and industrial partners, respectively. To advance beyond these tools will again require an effort spanning resources in academia, the national laboratories, and industry.

DOE has a long history of engagement with the combustion science and technology community. In 2006 the Office of Basic Energy Sciences convened a workshop on Basic Research Needs for Clean and Efficient 21st Century Transportation Fuels.[3] That workshop identified a single grand challenge: the predictive simulation of internal combustion engine performance in an evolving fuel environment. More recent engagement with academia, national laboratories, and industry (Chrysler, Ford, GM, Cummins and Caterpillar) over the past year has identified two specific simulation targets, achievable in the next five years, which will enable industry to realize substantial gains in efficiency, greater than 20% beyond current state-of-the-art engines.

First, the simulation, understanding, and control of the inherently random turbulent mixing and chemistry of combustion, so-called stochastic in-cylinder combustion processes, must be addressed. While present in all combustion engines and generally accounted for with generous design margins, these processes lie on the critical path to developing new combustion technologies and realizing fuel-efficient, clean, high-power-density, down-sized engines and can no longer be conveniently marginalized through conservative design. Second, modern engines require the control of fuel sprays in an evolving fuel environment that is far more subtle than that needed for earlier engines and that can be obtained only through predictive modeling and simulation. Both of these targets can be achieved with the targeted application of high-

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[3] http://science.energy.gov/~/media/bes/pdf/reports/files/ctf_rpt.pdf

performance, massively parallel computing through the evolution of existing codes that scale to the full size of current leadership-class machines.

The Workshop to Identify Research Needs and Impacts in Predictive Simulation for Internal Combustion Engines (PreSICE) focused on these two near-term priorities. The PreSICE workshop brought together 63 participants from government (16%), industry (25%), academia (35%), and the national laboratories (24%) on March 3, 2011, in Arlington, Virginia to develop a community consensus on the research needs and potential impacts of a focused DOE-led effort to create the next-generation predictive simulation-based design tools for engines. The charge to the PreSICE workshop can be summarized as seeking the answers to four basic questions:

1. Why is an investment in a pre-competitive, academic–lab–industry partnership for the development of predictive combustion simulation for engines needed?
2. Why is now an opportune time to develop simulation tools for advanced engine design?
3. What are the critical needs in basic and applied R&D in chemistry, physics, and engineering required for the successful realization of predictive combustion simulation for engines?
4. What is the potential impact on the U.S. automotive and engine industries if new simulation tools are developed?

The balance of this report summarizes the consensus of research needs from breakout groups on the two priority areas and defines the benefits of implementing a PreSICE research and development program.

Strategic Focus Areas for PreSICE

Strategic Focus Areas for PreSICE

During a series of small workshops in 2010, the U.S. gasoline and diesel engine manufacturers identified barriers in the understanding and control of sprays and stochastic in-cylinder processes as representing the most significant impediments to enhanced engine efficiency. Several other critical areas were also identified where predictive modeling could play an important role, including chemical and physical processes at surfaces, high-pressure dilute-combustion phenomena, and near-wall processes. At the PreSICE workshop, participants were asked to focus on the highest-priority areas utilizing breakout panels in each area.

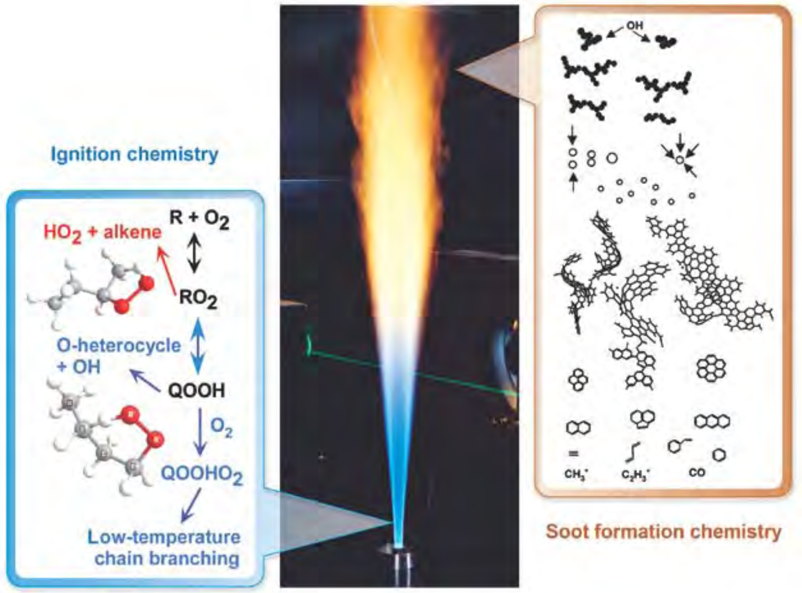
All advanced engine technologies with the potential for significantly improved fuel efficiency over engines dominating the road today will have fuel directly injected into the engine cylinder as a spray. Since the injection process determines initial conditions for both real engines and simulations, the lack of accurate fuel spray models is a major barrier to rapidly designing and introducing these clean, high-efficiency engine technologies, especially in an emerging diverse-fuel source future. The entire cascade of processes including orifice flow and cavitation, atomization, dense secondary breakup, dilute spray dynamics, and vaporization needs to be accurately modeled in order to characterize these initial conditions. Developing these tools is an essential first step toward the goal of a complete, predictive simulation capability for engine design and optimization. Standing alone, these tools can significantly shorten the engine development cycle, increasing our industrial competitiveness and helping us to get cleaner, more efficient vehicles into the market more quickly.

The maximum fuel efficiency of advanced engine technologies is often achieved near the extreme limit of combustion stability. Thus, engine performance is frequently constrained by intermittent stochastic events that lead to poor combustion, knock, or misfire. The coupled physical and chemical processes causing these events span a wide range of time and length scales, and current engineering design codes cannot capture these phenomena. Without the capability for predicting flow and mixing processes leading up to these events, engine design and calibration require significant levels of trial and error and must be made more conservative, thereby sacrificing fuel efficiency. The ability to predict and minimize cyclic variability and more rapidly optimize and design engines will have a significant positive impact on fuel economy, emissions, and the marketability of advanced high-efficiency mainstream propulsion devices [e.g., direct-injection, stratified-charge spark-ignition (DISI) and homogeneous-charge compression-ignition (HCCI) engines]. Achieving this goal will be an initial step in a larger program vision aimed toward developing fully predictive models for all engine air and fuel flow, fuel–air mixing, combustion, and emission processes. These models will be required in order to design dramatically advanced, clean, high-efficiency engine technologies for an evolving fuel environment. The advanced engines will help the U.S. meet goals of reducing oil use, lowering CO_2 emissions, and improving air quality.

Engine combustion involves turbulent flows and a variety of complicating factors. These factors include highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing, turbulence–chemistry interactions, compressibility effects (volumetric changes induced by changes in pressure), and variable inertia effects (volumetric changes induced by variable composition or heat addition). Coupling between these processes occurs over a wide range of time and length scales. Further complications arise when multiple phases are present due to the introduction of dynamically evolving interface boundaries and the complex exchange processes that occur as a consequence. At the device level, high performance, dynamic stability, low pollutant emissions, and low soot formation must be achieved simultaneously in a complex, highly confined geometry that generates extremely intricate flow patterns. The flow and combustion processes are highly turbulent (i.e., integral-scale Reynolds numbers of 100,000 or greater), and the turbulence dynamics are inherently dominated by the device geometry and operating transients. In many cases, operating pressures approach or exceed the thermodynamic critical pressure of the fuel, which significantly alters its thermodynamic and transport properties.

The underlying chemistry of combustion is both complex and non-linear. A chemical kinetics reaction set that includes all reactions relevant to even a model fuel such as octane includes hundreds of chemical species and thousands of individual reactions. A complete description of a complex fuel such as gasoline would be larger by a factor of ten or more.

Where does chemistry matter in combustion?



Combustion is an intricate web of interrelated chemical and fluid mechanical phenomena. The nineteenth-century inventors of internal combustion engines, such as Otto and Diesel, knew only that burning fuel gave heat. Indeed, the heat released by chemical reactions powers the combustion process, and designing today's engines requires predicting heat release with a precision unimagined by Otto or Diesel. Furthermore, in modern engines performance is always conditional on meeting increasingly stringent emissions limits. What are the areas where the details of combustion chemistry make a difference?

The forefront of combustion research depends on several key areas where performance is particularly sensitive to chemistry. For example, the modeling of pollutant formation requires accurate prediction of molecular species that occur at the part-per-million level or below in the combusting mixture. The nature and amount of pollutants—nitrogen oxides, particulates, partial oxidation products—depend on details of key individual chemical reactions. In addition, predicting the timing and location of the most fundamental combustion chemical property, heat release, requires an understanding of the complex oxidation chemistry that leads to autoignition.

This is especially true in advanced compression ignition engines or for stochastic events such as "megaknock." The path to autoignition depends delicately on whether crucial chemical reactions are producers ("chain-branching") or consumers ("chain-terminating") of reactive radicals. Most critically, the behavior of almost all of these chemical processes at very high pressures is inadequately understood. As clean, efficient engines move towards increased boost and higher operating pressures, fundamental knowledge about these areas of chemistry will be essential for accurate predictive simulation.

The timescales for these reactions span a factor of one million from the slowest to fastest. Strong overlap exists between the timescales for turbulent processes and these reactions, creating strong coupling between the chemical and turbulent elements of combustion. As a result of these combined factors, the computational cost of chemistry often limits the performance of combustion simulation codes. Indeed, to date no combustion simulation is capable of simultaneous high-fidelity chemistry and three-dimensional turbulence simulations under engine operating conditions.

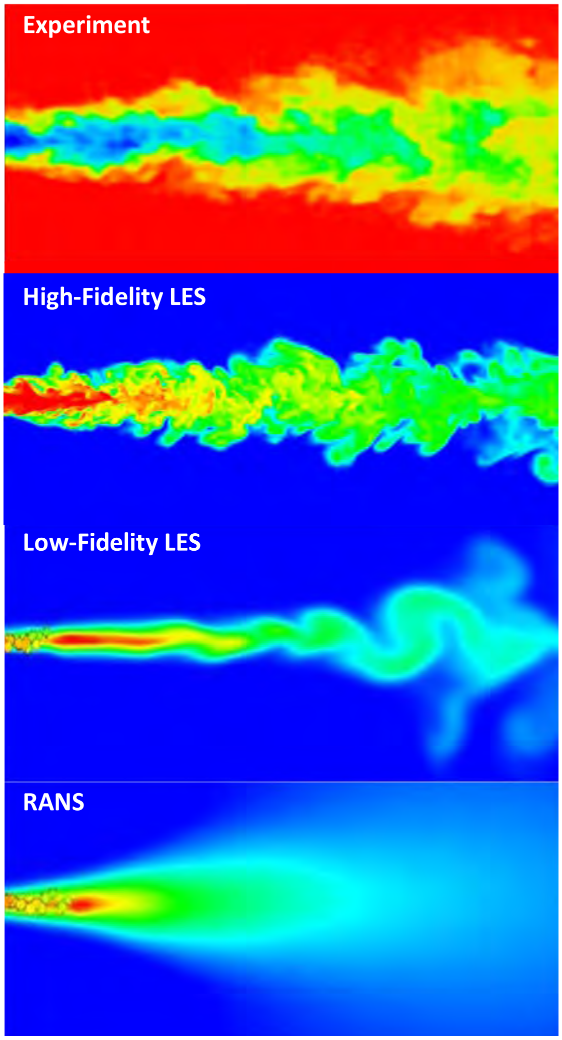
No single experimental or numerical technique is capable of providing a complete description of the processes described above. The highest-quality experimental diagnostics provide only partial information. Modeling and simulation of these processes will always be limited by computational power. To this end, physical models and numerical algorithms that address critical engine combustion processes must be developed and implemented using a hierarchy of tools. Three levels of computational fluid dynamics (CFD) techniques are relevant: direct numerical simulation (DNS), large-eddy simulation (LES), and Reynolds-averaged Navier-Stokes (RANS) approximation. DNS, LES, and RANS provide different degrees of solution fidelity in capturing the underlying physical processes. Higher fidelity (i.e., resolution in space and time) corresponds to higher computational requirements.

By definition, DNS provides an exact representation of the governing equations without the need for modeling. However, the computational requirements are extremely high. In practice, even with the largest supercomputers envisioned in the next twenty years, DNS cannot be applied to a full engine geometry or component at the relevant operating conditions. DNS does have an important role to play for canonical simulations aimed at physics discovery related to small-scale turbulence–chemistry interactions. The goal is to isolate and quantify important physical interactions in a manner that contributes to the development of models used for LES and RANS.

At the other extreme, RANS employs filtering in time to derive the governing equations for the mean state. Turbulent interactions over the full range of dynamic scales are completely modeled to make the calculations affordable for engineering analysis. However, only the largest energy-containing features in a flow are resolved and no information exists to describe interactions between the small scales. As such, the computational requirements for RANS are relatively modest. A RANS simulation of a complete single engine cycle requires less than one day on moderate-sized computing clusters that are available to industry and universities. RANS has been used effectively to design aspects of conventional engine combustion systems. However, since turbulent fluctuations are not resolved with these codes, physical processes such as cycle-to-cycle fluctuations and turbulence–chemistry interactions happening at the smallest scales cannot be predicted and a case-by-case calibration of models is required to account for the unresolved physical processes in a given engine system. This constraint severely limits the range of combustion challenges for which RANS can be utilized because predictions are only reliable in a regime that has already been tested and validated.

LES bridges the gap between DNS and RANS in fidelity and computational requirements. It can be performed for a range of resolutions from near-DNS to RANS-like. As in RANS, modeling is required to account for unresolved small-scale physical processes. However, the models do not need to represent as much unresolved physics as do RANS-based models. Moreover, the burden

Success requires a hierarchy of codes



This figure shows qualitative images of various fuel sprays at different levels in the computational hierarchy in terms of fidelity. At the top is an image of a spray from an experiment showing complex, unsteady behavior. This level of detail can also be achieved by direct numerical simulation (DNS) for simpler flows, although not realistic engine sprays. The second image down shows a fuel jet modeled using high fidelity large eddy simulation (LES), which approaches DNS. This captures most of the flow features using dense computational meshes. The third image shows a fuel spray using a lower fidelity LES. This level uses a coarser grid that requires less computational resources but still captures the larger aspects of the spray structure, including its unsteadiness and potential stochastic behavior. The final image at the bottom shows a diesel spray represented by a Reynolds averaged Navier-Stokes (RANS) calculation, the least computationally expensive method. At this level, only the mean or average aspects of the spray are captured.

This hierarchy provides a foundation for several important aspects of predictive combustion simulation. The upper levels of the hierarchy can be used for discovery to understand the physical and chemical processes that are important for engine modeling. They can also be used to provide insight for model development and data for model validation at the lower levels. This greatly improves the modeling accuracy at the lower levels which have a greater reliance on model tuning but are more readily used in engine design because of lower computational costs.

on the models decreases with increasing resolution. As such, LES is well suited to capture the unsteady spray dynamics and cycle-to-cycle variations that have been identified as a principal obstacle to realizing further reductions in fuel consumption and pollutant emissions from engines. For these reasons, LES is anticipated to be the principal focus of future research efforts.

The mathematical formalism associated with LES allows great flexibility in how it is applied. In addition to being a powerful tool for engineering, high-fidelity LES can also serve as a powerful tool for scientific inquiries into the structure and dynamics of high-Reynolds-number geometrically complex flows. Just as one chooses the resolution at which a photographic image is resolved, one can conceptually choose the resolution at which pertinent broadband features of a flow are resolved if models are available that accurately represent the range of physical and chemical processes that occur on scales smaller than the grid spacing. As the resolution is increased, the cost associated with a calculation increases, but the range of scales over which the sub-grid models must work becomes proportionately less and they tend to be more universal in character. The mathematical formalism of LES also facilitates use of powerful identities associated with filtering that eliminate the need for tuning constants in the model. Given these attributes, LES can be used as both a tool for basic research and engineering design. The former requires use of more sophisticated "science-based" sub-models. The latter requires extension to "engineering-based" models so that the application of LES can be made reliable and affordable in the engineering sector. Advancing the state of the art in these areas for internal combustion engine applications must involve both a short-term focus on improved RANS models for engineering and a concurrent long-term focus on development of LES as a next-generation engineering tool.

Given the many challenges and needs outlined above, advances in high-performance computing and the related numerical techniques are necessary, but not sufficient alone, to achieve the goal of improved predictive models. Coordinated experimental efforts must also be advanced simultaneously in a manner that is directly aligned with the core modeling and simulation goals. Targeted experiments aimed at the same strategic focus areas will provide both the benchmark data required for model validation and scientific insights at engine-relevant operating conditions. Requirements for these experiments must scale with the complexity and fidelity of the numerical work. As more small-scale structures are resolved in the computations, the experimental efforts will need to also provide data with adequate spatial and temporal resolution. Advances in laser-optical diagnostics are also necessary to provide quantitative data for currently inaccessible high-pressure conditions, at sub-millimeter spatial resolution, and frame rates of many thousand images per second; all of which are beyond current capability.

An integrated combination of simulations and experimental methods will provide an unparalleled opportunity to advance fundamental combustion science in a manner that will revolutionize the performance of combustion systems and provide new predictive design methodologies for a wide array of engineering applications. It will facilitate the application of peta- and exascale computational resources for rigorous science-based validation of models using data acquired from carefully selected target experiments. Once validated against experiments, the high-fidelity simulations offer a wealth of information beyond that which can be measured directly. The numerical data provides both a detailed description of intricately coupled processes not otherwise available, and information required to improve and/or develop advanced engineering models that provide the fast turn-around times required by industry designers. Significant improvements can be derived using an optimal combination of methods to provide enhanced accuracy and confidence in a wide range of models and modeling approaches.

Each of the strategic focus areas, sprays, and stochastic in-cylinder processes is explored in depth below. Following is a description of the expected software tools and expectations for impact on future vehicles.

Strategic Focus Area: Sprays

All advanced engine technologies involve direct injection into the piston cylinder of liquid fuel as a spray (see the spray combustion processes insert on the following page). Fuel injection is a key controlling factor for engine performance and emissions and adds significant degrees of freedom—and complexity—to the design optimization process. Lack of accurate models hinders the design of optimized, clean, high-efficiency engine technologies. Advanced models for sprays will provide the foundational basis for accurate predictions of fuel–air mixing and combustion in a manner that significantly shortens design cycles.

Three focus areas have been identified in the broad context of sprays and multiphase flow for internal combustion engines. These are treatment of:

1. Fuel-delivery systems (internal flows inside fuel manifold and injectors),
2. In-cylinder fuel-preparation strategies (fuel injection, mixing, and combustion), and
3. In-cylinder fluid–wall interactions and heat transfer.

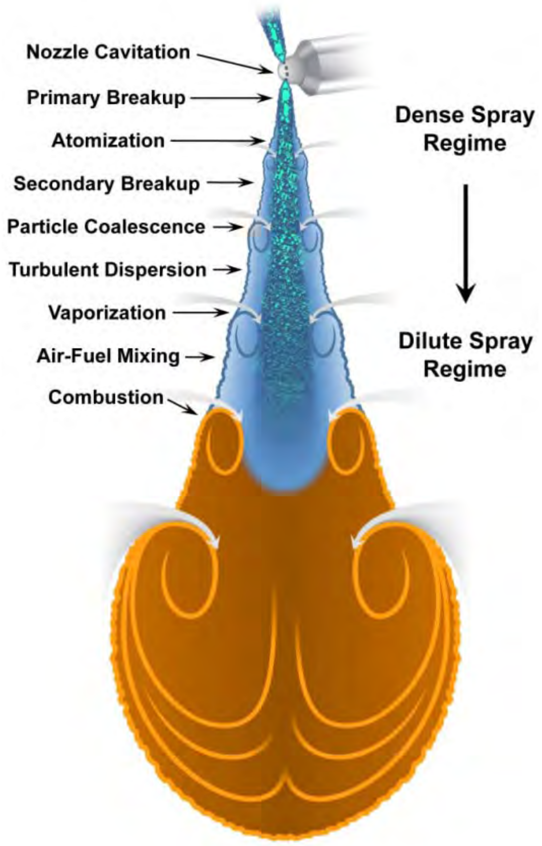
Processes associated with these are inherently coupled, but distinct in terms of model development and validation needs. In all cases, enhanced fidelity is required in the treatment of the unsteady, transient nature of the flow. The complexities associated with a variety of conventional and alternative fuels must also be taken into account.

Fuel injection involves a cascade of complex processes

Simulation of spray combustion processes in internal combustion engines poses a variety of challenges. Inherently, flow inside the cylinders involves extremely complex interactions between the injected liquid fuel, air, and combustion products. Liquid fuel is injected into a high-pressure environment, which often exceeds the thermodynamic critical point of the liquid. The way in which the fuel is injected and resultant interactions with the in-cylinder gases can have a profound effect on engine performance and emissions.

Complex interactions induce primary breakup of the liquid jet, which is followed by atomization and secondary breakup of the fuel into drops. The heterogeneous spray evolves as a complex distribution of fuel drops that interact with both the turbulent gas mixture and other drops. Interactions include deformation, collisions, and coalescence. Millions of individual drops continue to get smaller, more dispersed, and more dilute through a cascade of vaporization and mixing processes. Ultimately the fuel–air mixture reacts and combustion occurs to provide power.

How combustion occurs is controlled by the resultant exchange of mass, momentum, and energy between the gas and liquid. This process is complicated by additional factors such as spray–wall interactions and the related impact on heat transfer. Modern simulation tools and established theories do not currently exist that accurately describe these details with the required fidelity for advanced designs. Thus, development of advanced spray models requires new theoretical and numerical treatments along with companion experiments to provide the data required for validation.



Spray Focus Area 1: Fuel Delivery Systems

Fuel delivery systems associated with direct-injection engines operate at extremely high pressures and involve complex internal flow processes. Flow transients in the “common rail systems” that feed fuel to the injectors can significantly affect the cycle-to-cycle characteristics of individual injectors and the resultant in-cylinder processes. The mechanical characteristics of the injectors themselves can impose variations in the injection process as well as turbulent flow and cavitation within the injector nozzle. In addition, subtle geometric flaws associated with manufacturing of injectors can impose significant uncertainties and cycle-to-cycle variations. Predicting the presence of cavitation and understanding the transient nature of both the common fuel rails and fuel injector needle dynamics will provide increased durability limits with respect to manufactured hardware as well as reduced design cycle times with optimized performance and emissions.

To develop accurate models of the fuel-delivery processes, current experimental capabilities must be improved by developing innovative methods that track the fluid dynamics within actual commercial fuel-injectors and nozzles. Current experimental techniques to probe these physics include the use of *x*-ray measurements to visualize needle movement and cavitation bubbles inside injectors, and constructing scaled-up or real-size, optically accessible injector nozzles to visualize cavitating flows. Most of this work has focused on characterizing cavitation phenomena because it is poorly understood how injector design and operation affect these processes. Furthermore, it is not understood how these processes influence spray break-up and atomization processes as the fuel reaches the injector nozzle exit. Finally, unresolved questions regarding the applicability of current measurements exist because cavitation processes do not scale, which limits the translation of knowledge from scaled-up nozzle experiments.

Spray Focus Area 2: In-Cylinder Fuel Preparation

Fuel preparation both in terms of the injection timing and strategy—e.g., single-pulse or multiple-pulse injection, subsequent in-cylinder mixing, and the resultant combustion processes—involve a wide variety of strongly coupled multiphase processes. From the more classical perspective, treatment of liquid injection, primary breakup, atomization, and dense spray dynamics (sheet, filament, and lattice formation) outside the injector nozzle is still largely empirical and requires significant model development. Descriptions of secondary breakup, particle deformation, and coalescence processes are equally empirical in nature. This combination of empiricism imposes significant uncertainties that limit the accuracy of current simulation techniques. In the dilute spray regime, drop dynamics, vaporization, and combustion have been more accurately treated, but several modeling issues still exist. Advanced treatment of two-way coupling between the gas and dispersed-liquid phase is required as well as treatment of turbulence modulation (damping of turbulence due to particle drag effects) and turbulence generation (production of turbulence due to particle wakes) effects. Finally, multiphase combustion models must incorporate the coupled effects of all of the processes listed above to achieve a more refined predictive capability.

In addition to improved models for classical spray phenomena, models that account for thermodynamically near-critical and supercritical flow processes must also be considered in the context of fuel-preparation strategies and the resultant in-cylinder flow dynamics. Many advanced engine concepts now employ cylinder pressures that exceed the thermodynamic critical pressure of the fuel at the start of injection. For this situation the classical view of spray atomization and secondary breakup processes comes into question. Instead, injection occurs at "transcritical" conditions, where the fuel is supercritical with respect to pressure and subcritical with respect to temperature. Under such conditions, substantial thermodynamic non-idealities and transport anomalies exist. Mixture properties exhibit liquid-like densities, gas-like diffusivities, and pressure-dependent solubilities. The isothermal compressibility and constant pressure-specific heat increase significantly while the heat of vaporization and the surface tension diminish. This combination significantly alters subsequent in-cylinder mixing and combustion processes and must be rigorously understood. Treating these processes also has direct relevance to the use of alternative gaseous fuels such as natural gas or hydrogen, which are injected at extremely high pressures to boost energy densities of the fuels and thus performance.

To move beyond empirically based spray models, experiments must also push beyond a limited range of spray regimes (namely, the dilute limit) toward providing a complete description of these flows over a wide range of thermodynamic conditions. Techniques must be developed that provide a complete temporal and spatial history of fuel properties during transient injection operations at conditions when cavitating or flash-boiling phase transformations are present. Measurement techniques are needed to probe flow velocities, pressure, temperature, and vapor fraction. Current *x*-ray techniques can provide detailed measurements of injector needle movement, bending, and bouncing, but experiments must also be designed to link these processes together to provide an understanding of how fuel flows are influenced by these needle movements. Also, measurements are needed that simultaneously probe cavitating flows and their propagation into spray break-up and atomization processes. All of these measurements need to occur under real operating conditions (e.g., over the full range of relevant pressures), with real injector geometries.

In the near-nozzle dense spray region, measurements are needed that can spatially and temporally resolve the physics of primary atomization processes. Resolution of these physics poses significant measurement challenges due to high optical densities (inaccessible to typical laser diagnostic techniques), small length scales (on the order of microns), and high velocities (on the order of 300–400 m/s for modern diesel injections). High-resolution high-speed imaging techniques are needed that can resolve the development of surface waves, ligaments, and drops. It is also necessary to develop diagnostics capable of penetrating the optically dense liquid core to quantify velocities and liquid volume fraction. Current *x*-ray techniques can quantify fuel mass fraction in these regions, but progress must be made towards single-shot capability so that transient injections effects can be quantified.

Downstream of the dense spray region, full-field mapping of drop sizes, drop and gas-phase velocities, and liquid and vapor volume fraction measurements are required. Current diagnostics for drop sizing are fairly mature, but are limited to specific drop size ranges and limited to point measurements. Full quantification of sprays will require the development of full-field spatial resolution with the capability to measure a wide range of drop sizes. Measurements of the fuel–vapor distribution are also required to validate vaporization processes. A key challenge will be to develop techniques capable of probing a variety of conventional and alternative multicomponent fuels.

Spray Focus Area 3: In-Cylinder Fluid–Wall Interactions

The final focus area involves treatment of in-cylinder fluid–wall interactions and the related heat transfer processes. Regardless of the mixture preparation technique employed to achieve optimal combustion, fuel impingement and thermal stratification caused by necessarily cooler surfaces can impose significant losses and/or degradation of performance and emissions characteristics. It also can induce undesirable friction and wear on various components. Treating the coupled effects of fluid–wall interactions, both in terms of the effects on the mixture and heat transfer, is an imperative part of the design process. Current models fail to capture important transient and unsteady phenomena that can lead to poor uniformity in cooling and undesirable combustion characteristics.

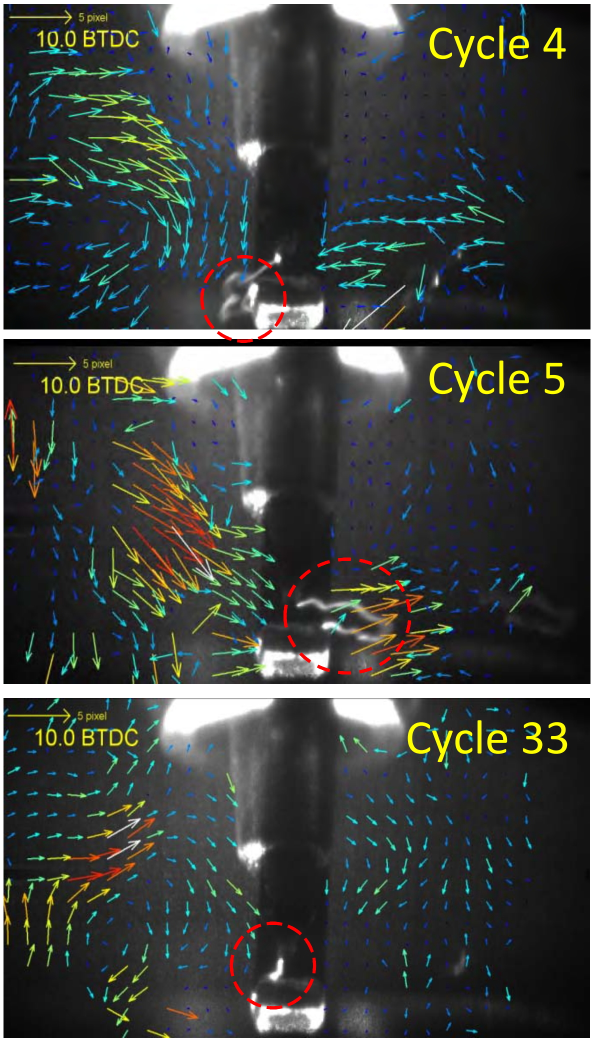
To quantify spray–wall interactions, current measurements of spray impingement need to be extended to include oblique impingement angles and complex surface geometries. In addition, measurement techniques will be required that can quantify droplet velocities and geometries during impingement, splashing, rebound, and sliding along wall surfaces while tracking the entire temporal history and potential outcomes of drop–wall interactions. Fuel film thickness measurements need to include speciation due to multicomponent fuels and temporal histories as film vaporization occurs. Measurements to quantify the interaction of droplets with existing fuel and oil films are also needed. Ideally, these measurements should be performed under real operating conditions so that the influence of transient ambient conditions and piston motion can be understood and quantified. An additional key component for the development of accurate fuel–film and spray–wall interaction models will be to measure transient wall temperatures and heat transfer rates.

Strategic Focus Area: Stochastic In-Cylinder Processes

Advanced engine combustion technologies are being developed that promise significant increases in fuel economy while maintaining low emissions. However, engines are sufficiently complex that every combustion event and every fuel-spray injection event is different. Moreover, the intrinsic instabilities associated with turbulent flow cause fluctuations of in-cylinder conditions even for nominally similar starting points. For advanced concepts such as lean-burn-stratified-charge and homogeneous-low-temperature combustion, these fluctuations and cycle-to-cycle variations can result in intermittent, currently unpredictable poor combustion events such as misfires or incomplete burns. Although these events may occur only once in every 1,000 to 10,000 cycles (once per minute to once every few minutes), they nonetheless can significantly degrade engine performance, increase emissions, or even damage the engine. Because these events cannot be reliably predicted, engine developers must allow large margins of safety to maintain performance and meet regulations. This tradeoff results in an unnecessary sacrifice in the true efficiency and emissions potential of a new engine.

For these reasons, a critical focus is stochastic in-cylinder processes. Here the term “stochastic” embodies the following aspects of in-cylinder combustion: the flow and combustion events are not repeatable from one engine cycle to another; the root causes of this variability are not well understood; the deviations from the mean or average engine cycle can be large; and rare events that occur as infrequently as one cycle in several thousand can be important. The results of these off-normal events may include incomplete combustion that raises pollutant levels above acceptable limits or pre-ignition engine “knock” with the potential to damage an engine.

Winning the engine lottery: controlling cycle-to-cycle variation in engines



Modern laser-based imaging technology enables photography inside of operating glass engines to visualize and quantify the effects of what is called cycle-to-cycle variations. This figure shows the same moment in three different engine cycles during spark plug firing. The arrows indicate the direction and the magnitude of the flows around the spark plug (center of the image) measured with a technique called particle image velocimetry. Clearly the flow looks different in every cycle. The spark plasma is shown by the thin white streak at the spark plug, highlighted by the circle. If this spark plasma is blown to an area where there is not enough fuel, combustion cannot start and the engine may misfire. (Figure courtesy of General Motors)

The operation of internal combustion engines requires carefully timed filling of the cylinders with air and introducing fuel to achieve mixing conditions that guarantee the desired high efficiency and low pollutant combustion. However, even though the mechanical movement of pistons and valves repeats perfectly, the detailed description of the way air and fuel enter the cylinders, mix, and burn varies from cycle to cycle. Over the average lifetime of an engine the number of fired cycles is on the order of the number of people living in the United States of America, about 300 million. Just as with people, none of those 300 million cycles are identical; they have a lot in common, but they exhibit noticeable differences that affect engine performance.

Engine designers strive to build engines that minimize the occurrence of strong cycle-to-cycle fluctuations to ensure the highest reliability possible and to enable operation of engines under conditions that maximize efficiency and minimize harmful emissions. Current designs function far from the limits of performance to control these fluctuations. To advance beyond the current state of the art, future engine designs must run under conditions that are beyond the limits of reliable operation. Greater control of cycle-to-cycle variations will enable the realization of these designs. Therefore, understanding the origin of cycle-to-cycle variations is crucial so that they can be reduced to the physical limit, given by nature and not by sub-optimized engine designs.

Three focus areas have been identified that address the needs for improved modeling of stochastic in-cylinder processes: (1) establish and characterize the underlying physical causes of stochastic events; (2) develop physically based CFD models that can be used to predict and control variability; and (3) quantify and manage the propagation of uncertainty or fluctuations in model parameters and boundary conditions on model predictions. There are coupled needs to these three areas for new and enhanced experimental platforms, diagnostic tools, and analysis methods that are required for discovery and validation measurements.

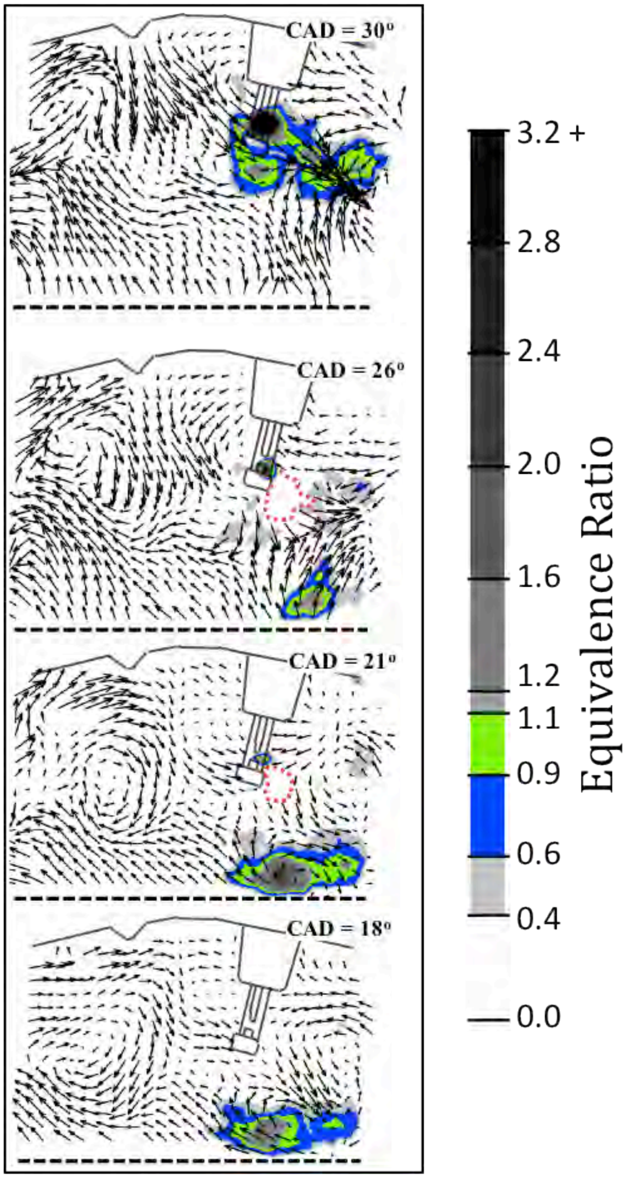
Stochastic Processes Focus Area 1: Physical Foundations of Stochastic Processes

The predictive power of any model relies on the accuracy of its description of fundamental processes. However, the underlying fundamental physical and chemical mechanisms for many intermittent or stochastic events in engines remain unclear. One example is pre-ignition or "mega-knock," which is a particularly damaging early ignition of the fuel–air charge. Large safety margins must be included in the design of advanced turbocharged spark-ignition engines to ensure that mega-knock never occurs, because the nature of these events and the factors that trigger them are not well understood. A second example is surface (wall) effects. A large fraction of cycle-to-cycle variability in emissions can be attributed to uncommon combustion events that take place at or near surfaces. However, heat transfer through deposits and chemistry near piston or cylinder walls are not well understood. A third example is high-pressure autoignition in advanced compression-ignition engines. Autoignition is highly sensitive to small variations in temperature and composition, and our understanding of chemical kinetics at high pressure is limited.

Advancing the fidelity and accuracy of predictive models that capture the range of stochastic in-cylinder processes will require investigating the root physical causes of transient phenomena. This investigation must incorporate "discovery" diagnostic measurements, and must also include fundamental theoretical and experimental studies of key processes. In this context, modeling at the highest level of resolution (DNS) can serve as a discovery tool.

It is critical to focus the efforts on identifying and understanding those physical phenomena that will have the greatest impact on improving predictive capability. In some cases, it may be possible to identify the areas that have the greatest potential (e.g., spray formation, turbulence–chemistry interactions, and pressure-dependent autoignition) through uncertainty and sensitivity analysis of the models. In other cases, even the basis for modeling is unknown, and the identification of relevant physical and chemical processes must rely on the design and application of experimental diagnostics that are capable of characterizing these transient events. Time-resolved, three-dimensional imaging of flow and combustion processes will be a critical need for discovery in this arena. Development of common platforms, amenable to detailed modeling, in which these diagnostics can be applied in multiple laboratories, will be important to accelerate progress. The challenges of such measurements are exceptional. Not only are significant breakthroughs needed before fully 4D-capable measurement tools of multiple parameters are possible; well-controlled experimental facilities that can provide reliable and repeatable starting and boundary conditions for benchmark experiments are of paramount importance.

Highlighting combustion with laser diagnostics



High-speed movie sequence showing the airflow (arrows) and the fuel distribution (color map) near the spark plug shown in the upper right of each frame. The colors highlight the regions where an ignitable fuel–air mixture is present. The area outlined by red dots is a starting flame but as the image sequence shows, this flame does not find enough fuel to continue combustion. This engine cycle misfired. (Volker Sick, The University of Michigan)

New phenomena discovery and model validation in engine combustion studies require detailed measurements of temperature, chemical species concentration, and velocity. Ideally, these measurements should provide the desired information in the form of a high-speed, three-dimensional movie. This is important because no two engine cycles are the same. Thus, snap shots taken in different engine cycles cannot be used to fully understand the stochastic nature of in-cylinder behavior.

Current camera and laser technologies allow capturing high-speed movies of mixing and combustion processes at the rate of thousands of pictures each second. This process is similar to the slow-motion movies we know from sports events with the major difference that laser methods allow us to see specific molecules or the motion of gases. This principle, for example, can be used to simultaneously measure the motion of gases and the distribution of fuel around the spark plug in an operating engine. The figure at left shows an image series that was captured in a direct injection engine to identify the causes of rare misfires.

Even 2-D measurements present significant challenges because thousands of images must be collected with separations of only millionths of a second. These requirements challenge the temporal resolution, sustained acquisition capability, and image processing capabilities of modern laboratories. Future developments will enable full 3-D cinematic imaging capability, further stressing experimental and analytical capabilities by a factor of ten or more.

For thorough investigation of the root causes of mega-knock or other uncommon but harmful events, multiple parameters must be quantitatively and simultaneously measured, with high temporal and spatial resolution, continuously over many engine cycles. The ideal diagnostic tools must be able to interrogate multiple fundamental parameters (e.g., heat release, flow velocity, temperature, fuel–air ratio, chemical composition) concurrently. Because correlations between two or more of these factors are expected to be critical for understanding stochastic events, separate measurements of individual parameters will not be sufficient.

Focused investigation on the key processes (e.g., hydrodynamics, heat transfer, high-pressure combustion chemistry) will involve detailed theory and computation anchored to accurate experiments. These studies should aim not simply at a more detailed description of elementary processes, but at delivering general models that can be incorporated into the full hierarchy of predictive simulation tools. Both theory and experiment must extend from single interactions or chemical reactions to their incorporation into CFD-based models. Carefully designed experiments that can isolate important aspects of the overall combustion process will guide and validate the fundamental theory and modeling. For example, experiments that quantify the response of a reacting flow to controllable local perturbations in temperature, pressure, or composition would both constrain models of transient phenomena and uncover hidden causes for non-reproducibility. Particular challenges in this context include the need to perform such experiments under conditions that are outside of currently explored values of pressure, temperature, and composition.

Stochastic Processes Focus Area 2: Models that Comprehend Variability

Current computer simulation models are satisfactory for capturing average or mean combustion behavior. Even there, the models require extensive calibration, and the calibration is limited to a narrow range of operating conditions. Current CFD models do not capture cycle-to-cycle variability and other stochastic events at all, and cannot be used to reduce or control variability. New design tools must be devised that explicitly account for variability. Direct calculation of in-cylinder turbulent combustion at full temporal and spatial resolution (DNS) would require computing power that is well beyond anything that is currently available or that will be available within the next ten years. Therefore, methods must be devised that allow calculations to a specified spatial resolution (the grid scale), and that incorporate physical models that account for the unresolved (“sub-grid” scale) phenomena. A new generation of physics-based, validated models for sub-grid effects is needed to increase the precision of engine design and to realize the maximum fuel economy benefits. Sub-grid models must account for interactions of multiple physical processes including liquid fuel sprays, turbulence, chemical reactions, and wall effects.

In some cases, the fundamental physical mechanisms underlying intermittent or stochastic behavior are understood. This is the case for some hydrodynamic instabilities, for example. Even in these cases, however, it is not necessarily clear how to translate this physical understanding into a sub-grid model. Improving the sub-grid models requires a more detailed description of the physical processes and experimental data for validation. The associated research must include highly accurate, quantitative measurements of sub-grid phenomena. This will be facilitated by the establishment of well characterized, highly controllable experimental platforms, for which corresponding simulations can be carried out at the highest resolution possible. Optical, and in particular laser-optical measurement technology, is, in principle, suitable for such experiments. However, adaptation to high pressures, high temperatures, and the transient conditions present in combustion engines requires substantial advances in high-speed and high-resolution measurement capability.

Spot the difference: How are experiments and models compared?

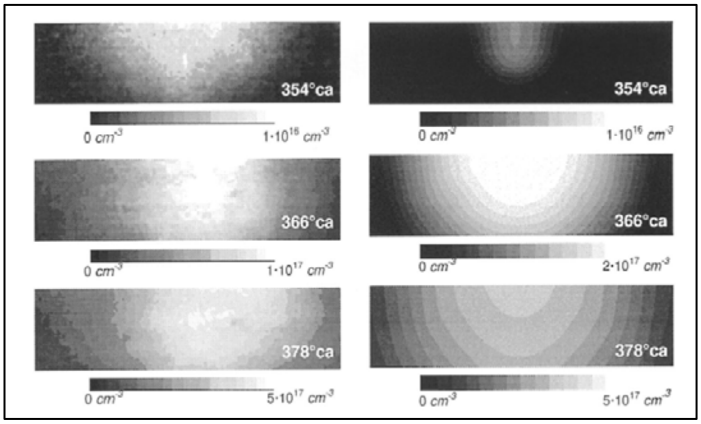


Figure 1. *Experimental and modeling results of the averaged distribution of nitric oxide, an important pollutant, in a gasoline engine. (Josefsson et al., 27th Symp. (Intl.) on Combustion, 1998)*

The reliability and accuracy of predictive modeling tools must be confirmed through thorough validation tests against a wide range of experimental results. The output of averaged modeling results such as those obtained with currently used computational fluid mechanics tools can easily be compared to experimental data with a "spot the difference" approach. An example is shown in Figure 1.

However, such an approach will fail for the predictive tools that are envisioned for the future where individual engine cycles will be resolved. Individual engine cycles will never be exactly like any other cycle (see sidebar: "Winning the engine lottery: controlling cycle-to-cycle variation in engines"). Likewise, the result of a simulation that resolves individual cycles will never be exactly like experimental results. New analysis tools must therefore be developed and adopted to internal combustion engine research that allow comparisons of model predictions with experimental results.

An example of such a tool is Proper Orthogonal Decomposition (POD). This mathematical technique extracts common features, or "modes," from experiments and models and then allows a quantitative assessment of similarity between the two. Utilized in other areas such as facial recognition, this technique is fairly new to engine research but has shown promise, as illustrated in Figure 2.

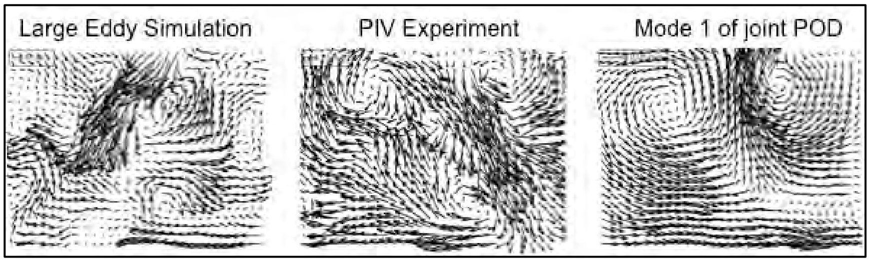


Figure 2. *Flow field structures from individual cycles have a very different appearance. A comparison of an LES flow field (left) with an experimental result is therefore very difficult. POD techniques enable rigorous comparison by extracting underlying structures (right) that are common to all data along with a number that shows their importance for each cycle (Courtesy of V. Sick, The University of Michigan).*

These advances include both the physical foundations to quantify the measurement signals and new developments in laser sources and detector technology. The experiments and simulations provide both a discovery platform to establish the proper physics foundation for sub-grid models and detailed data for verifying model formulations. Hydrodynamic, thermodynamic, and chemical parameters can be systematically varied over engine-relevant ranges to ensure that the models have the proper physical formulations, accuracy, and relevance. This level of investigation will feed into the hierarchy of models that successively move to lower resolution and computational time but increased reliance on sub-grid models, as discussed above. Each level of modeling provides a test and validation platform for lower-resolution modeling. This provides the required systematic path to reduce the uncertainty in models so that they are better able to capture stochastic events. Final validation of the models will require comparison to engine experiments that are targeted at stochastic events.

Simulations of engine combustion require large chemical kinetic mechanism models to predict autoignition and pollutant emissions, for example. Chemical kinetics often dominates the computational effort. To mitigate this, sophisticated methods for efficient numerical use of chemical models and for reducing the scope of chemical mechanisms are necessary. Increasing the spatial resolution of a simulation (reducing the grid scale) often demands relaxing the resolution of the chemistry for the computation to remain tractable. For example, developing adaptive chemistry codes that can increase the complexity of the kinetics only where and when it is necessary in the calculations could minimize the computational burden while maintaining accuracy.

To address this issue, it is necessary to create methods that couple direct evaluations of chemically relevant small-scale processes such as elementary rate coefficients and transport properties at very high pressures into models that can be efficiently integrated into CFD codes. These methods may include a range of software tools employing rate-rules generation, automatic mechanism generation, and transport property generation.

Many areas of combustion chemistry encompass substantial uncertainty. The new methods and models will be aimed at those chemical processes that govern the response of the combustion system to stochastic conditions—the specific chemistry that turns a fluctuation into an undesirable or damaging combustion event. As noted earlier, advanced combustion technologies are expected to include much higher operating pressures than current engines. Understanding of combustion chemistry at high pressures is limited, and simulation of stochastic events may require new fundamental knowledge about chemical mechanisms that amplify the effects of variability in flow or composition.

Developing and validating models for stochastic processes will require new mathematical approaches. Model development would benefit from new theoretical frameworks and numerical approaches for addressing such issues as turbulence interaction with sprays and combustion, and with wall boundary layers and heat transfer. Validation of models designed to capture stochastic events will require advanced tools to describe time- and length-scale correlations, cross correlations, and other spatial descriptions such as proper orthogonal decomposition. The advanced analysis methods will be required to effectively process experimental and simulation results so that causes of stochastic processes can be understood and control strategies can be developed.

Stochastic Processes Focus Area 3: Accuracy and Uncertainty of Simulations

To meet the goal of reducing the design and calibration margins needed to ensure regulatory emissions compliance while maximizing efficiency and customer value, design tools must provide accurate descriptions of the combustion process. Moreover, minimizing stochastic variations in combustion performance requires that contributions of individual sources of inaccuracy and uncertainty must be clearly isolated and quantified.

Uncertainty in the predictions can be reduced by improving our knowledge of the underpinning physics and chemistry. Here we are concerned with understanding how the remaining uncertainties in the physical and chemical description of the process (e.g., energy dissipation and kinetic rate coefficients) and in the specification of initial and boundary conditions (e.g., fuel composition, engine inlet flows) propagate through the simulation to ultimately impact the accuracy of the predictions. The latter source of uncertainty can be particularly pronounced in simulations of engine transient response. At the same time, it is important to consider uncertainties that result from limitations in the computing resources that are available (e.g., spatial and temporal resolution, number of cycles simulated) and uncertainties that are inherent in the level of description that has been adopted (e.g., DNS versus LES versus RANS). To this end, research focused on the characterization of uncertainty should incorporate the following three main elements.

First, closely coordinated examinations of the strengths and limitations of each modeling approach should be performed by comparing predictions with well-defined target experiments performed on common platforms at multiple locations. Common platforms are essential to provide the required broad range of experimental data that could not be obtained in a single laboratory. Synergistic experimental investigations utilizing common test platforms are necessary in multiple laboratories with overlapping scope but different focus areas to increase confidence in understanding non-linear relationships between many variables that lead to stochastic behavior, which is too complex to be addressed in single, isolated experiments. Through this comparison, the impact of uncertainties in the physical and chemical descriptions of the combustion process and of the initial and boundary conditions on the accuracy of the simulation predictions will be clarified. An understanding of the resolution and level of physical description required to predict various aspects of the combustion process with sufficient accuracy will be developed by comparisons between predictions obtained using different formulations and levels of resolution.

Second, methods must be developed to understand the propagation of uncertainties within the hierarchy of simulation tools. Both global and local sensitivities of the simulations to these uncertainties must be characterized, and interactions among uncertainties need to be quantified. This understanding will be vital to developing confidence in predicting the engine response to variations of input parameters: fuel properties, for example. In some cases, this may require that improved or new uncertainty analysis techniques be developed. For example, the quantification and propagation of uncertainties in theoretical chemical kinetics calculations may be important, and this has not been thoroughly explored.

Finally, the introduction and propagation of uncertainties introduced by dynamic changes in the modeling and numerics must be examined and characterized. Examples include dynamic grid resolution changes, or on-the-fly kinetic mechanism reduction based on local thermo-chemical conditions. Development of these capabilities, and characterization of other aspects of uncertainty propagation, must be performed in the context of simulation tools that are developed to take advantage of modern advances in computer architecture that offer massive multithreading capability and complex memory hierarchies.

Expected Software Tools

New software tools that can accurately and reliably predict spray behavior and capture variability in the combustion event are critically important for the development and design of next-generation high-efficiency, low-emissions engines. Given the inevitable tradeoffs that exist between accuracy and computational cost, multiple levels of CFD codes must be advanced simultaneously. Industry codes for design must be advanced using affordable models based on RANS and/or engineering LES approaches and run on engineering-relevant computer platforms. At the same time, research codes that provide high-fidelity LES, and possibly DNS, and that run on the most advanced, massively parallel platforms are required to provide highly accurate computational benchmarks. Zero- and one-dimensional codes are also required for system-level analysis and optimization to substantially shorten the design cycle.

Table 1 summarizes the primary modeling needs and required supporting technologies. Detailed model validation will require simultaneous and complementary advances in experimental capabilities to provide both new technical insights and pertinent validation data.

Table 1. Primary needs for development of advanced spray and stochastic simulation technologies for internal combustion engines.

Hierarchical model development, validation and reduction
Benchmark optical and canonical experiments for validation and discovery
Companion high-fidelity LES for detailed model development and reduction (detailed physics)
Engineering LES/RANS for engine cycle optimization and analysis (fast solution times)
DNS for analysis of small-scale turbulence-chemistry interactions
Sub-model development—sprays
Injector internal flow dynamics
In-cylinder breakup and atomization
Multiphase flow and spray dynamics
High-pressure (supercritical) phenomena
In-cylinder impingement and heat transfer
Turbulent mixed-mode combustion
Sub-model development—stochastic processes
Engine-out emissions and soot
Detailed and reduced chemical kinetics
Sub-grid models for physics-based scaling
Mega-knock and autoignition chemistry
Boundary-layer flow and heat transfer
Analysis approaches for validation work
Tool infrastructure development
Advanced grid generation and grid quality assessment
Core solver development (science-based LES and engineering-based LES/RANS)
Advanced model reduction techniques and uncertainty quantification
Post-processing, visualization, data management for science and engineering

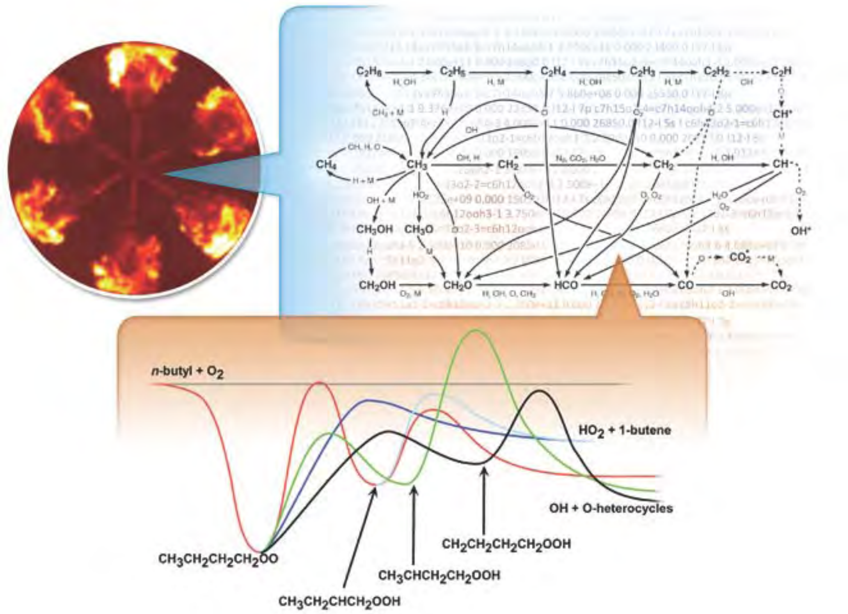
Modeling combustion chemistry: a hierarchy of complexity scales

At the highest level of detail combustion involves thousands of chemical species, participating in many tens of thousands of individual chemical reactions, each of which in turn has a detailed description in terms of fundamental physical principles. Just as in the fluid mechanical description of turbulence, the computational time and expense necessary to completely resolve the chemistry at the highest level is far beyond current or envisioned design tools. Therefore, a successful model of combustion chemistry must include a hierarchy of modeling strategies that can be adaptively applied in an overall simulation.

The calculation of elementary reaction kinetics from first principles is a discovery tool in the same way that DNS is a discovery tool for fundamental fluid mechanics. Rigorous quantum chemistry and theoretical kinetics reveal important details of the mechanisms of individual critical or representative reactions, knowledge that improves reliability for whole classes of similar reactions. To model full combustion processes, the pressure- and temperature-dependent kinetics are parameterized by simple functional forms that are employed in a "rate equation" that represents the individual reaction.

A comprehensive chemical kinetic mechanism collects such rate equations for all of the relevant chemical reactions. Evaluating even these rate equations for all the chemical reactions in a combusting mixture is usually too computationally intensive to carry out in conjunction with computational fluid mechanics simulations, so the mechanisms are usually further reduced in complexity, for example by eliminating species that do not significantly contribute to the target combustion property or by grouping species that behave similarly.

Predictive simulation of combustion chemistry must therefore choose the level of detail (complexity) that balances accuracy with calculation speed and computational expense. Making these tradeoffs wisely demands research to quantify the uncertainty of the underlying models and to rigorously manage that uncertainty through the simplification steps.



A hierarchy of chemical simulation tools is needed to address the challenges of advanced engines ranging from simplified mechanisms that execute quickly for use full engine simulations (upper left) to complex mechanisms that describe critical sub-processes such as pollutant formation (upper right) to fundamental quantum chemistry investigations of critical reactions (lower).

Current experimental facilities and related diagnostics do not effectively address the needs for model development in sprays or stochastic behavior at engine-relevant conditions. New experimental capabilities with well-controlled and characterized boundary conditions are imperative for developing quality benchmark data in several critical areas, including:

1. Measurement and characterization of internal nozzle flow regimes,
2. High-resolution temporal and spatial measurements of near-nozzle flows,
3. Measurements of drop-size distributions, composition and velocity in dense and dilute spray regimes,
4. Full-field temperature and fuel-vapor-fraction measurements,
5. Multicomponenent fuel vaporization measurements,
6. Techniques to characterize cycle-to-cycle variations, and
7. High-resolution temporal and spatial measurements of flow, ignition, and combustion.

Developing supporting infrastructure tools will be required for fast and routine implementation of various calculations. Both high-fidelity LES and engineering LES/RANS simulations require efficient grid generation techniques, including automatic grid generation capabilities and implementation of metrics to test grid quality. Efforts to systematically improve core solver algorithms and interfaces along with the serial and parallel performance in a manner consistent with the development of new computer architectures are also necessary. Advanced model reduction techniques, uncertainty quantification, and tools for post-processing, visualization, management of large data sets also will be required.

Computing and evaluating the kinetic mechanisms that govern the response of combustion chemistry to stochastic events will also entail new software tools. These must address the needs outlined in the Focus Areas for developing detailed mechanisms (e.g., methods for obtaining force fields, rate representations, rate coefficients, and rate-rule generation), for mechanism reduction, and for automatic mechanism generation. Software tools for both mechanism reduction and property evaluation at engine conditions must be developed and closely coordinated with improvements in CFD. These activities should be coordinated with complementary efforts that are currently underway elsewhere.

Given that multiple levels of modeling capabilities are required, models must be developed in a way that maximizes portability between different approaches. Supporting software related to uncertainty quantification is also required. A potential outcome will be the development of application program interfaces (APIs) or user-defined functions (UDPs) that facilitate portability between codes and platforms. The suite of validated models must be implemented in a manner that accounts for current and anticipated trends in computer software and evolving hardware architecture. While an open-source development model might potentially reduce barriers to collaboration at the pre-competitive research and development level, clear and timely benchmarks must be established to assess the utility of such an approach. To ensure the widest possible adoption by industry and maximum and timely impact on improving next-generation engines, new software must be readily adaptable to the CFD codes and related support infrastructure that will be used by industry partners.

Impact on Future Vehicles

Targets for future internal combustion engines include higher efficiencies (greater fuel economy) and lower emissions. Currently, the high end of thermal efficiencies in engines for conventional vehicles is approximately 30% for gasoline engines and 43% for diesel engines. Estimates for potential improvements are up to 45% for gasoline and 60% for diesel engines. These numbers represent significant fuel economy gains that could reduce U.S. fuel use for transportation from the current 13.5 million barrels of oil per day (MBOD) to less than 7.8 MBOD.

Advances in clean, efficient, and reliable engines

"Any sufficiently advanced technology is indistinguishable from magic," Arthur C. Clarke famously postulated. The engines of modern vehicles have reached this state for most consumers. In the middle of the twentieth century, many consumers had an all-too-intimate knowledge of the car's inner workings due to the requirement for frequent maintenance combined with the relatively simple nature of the engines. This was the era of the "shade-tree mechanic."

Today's engines employ the same fundamental principles, but execute them with more subtlety, control, and reliability. Today a computer terminal, not a shade tree, is needed to diagnose engine problems, and engines require less maintenance. Indeed, many of the adjustments made in tune-up 35 years ago are now handled by a computer in the car in real time. In the last 50 years dramatic advances have been made: the reduction of pollutants by over 99%, the doubling of power output for a given engine size, and the doubling of fuel efficiency.

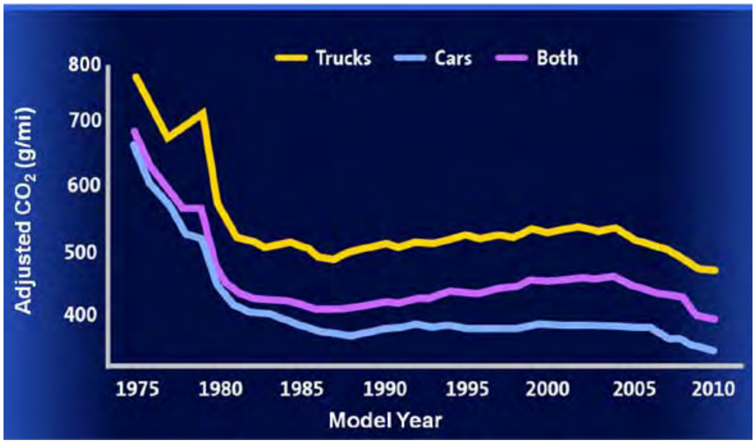


Figure 1. *Reduction in the CO_2 output of cars and trucks in the US per mile traveled showing a dramatic decrease over the last 35 years and recent acceleration of progress toward even lower emissions. (Figure courtesy of GM. Data from "Light-Duty Automotive Technology, Carbon Dioxide Emissions, and Fuel Economy Trends: 1975 Through 2010," EPA-420-R-10-023, November 2010)*

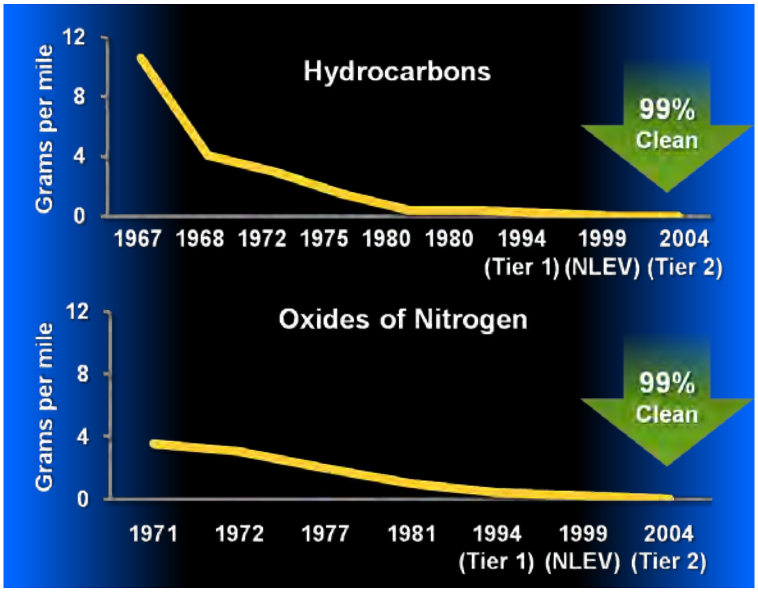


Figure 2. *Reduction in criterion pollutant emission standards. (Figure courtesy of GM)*

Current engine fuel economy and emission levels are already at the accuracy limits of modern modeling capabilities, largely because of the inability to predict undesired stochastic behavior. Therefore, the descriptions of combustion chemistry and how it is driven by other phenomenon in the combustion chamber, including turbulence and sprays, will need significant improvement to enable future, more stringent requirements to be accurately quantified and successfully met.

To increase the potential for generating expansion work in engines, an expected trend in future engine combustion-system development is higher operating pressures. At the same time, to lower emissions, higher levels of exhaust gas recirculation, low-temperature combustion, and lean combustion are anticipated to be required. To realize the advances, combustion phasing issues and issues of stability at high load must be overcome. All of these will require the inclusion of models for stochastic events into predictive tools to overcome their present limited ranges of applicability.

Future engines will also need to accommodate a wider range of fuels, including a variety of bio and bio-derived fuels. All of these will require kinetics descriptions in both full and reduced forms for accurate simulation. The speed with which such chemistries will be needed for future development programs will require improvements in the tools to quickly generate and reduce their reaction mechanisms, as well as the overall process by which this mechanism development is performed.

The goal of improved efficiency may also lead to innovative use of expanded engine cycles and architectures. Alternatives to traditional combustion-chamber designs have the potential to reduce thermal losses, for example. Such approaches would benefit from improved near-wall turbulence treatments to reduce uncertainties from the altered fluid mechanics and to provide more accurate predictions of wall heat transfer. In a similar vein, reducing flow losses in the intake ports would contribute to higher efficiency; this improvement also would be facilitated through improved turbulence treatments. Reducing the uncertainty of the charge composition at intake-valve closure from predictive CFD simulations would contribute to improved, more efficient engine designs.

Uncertainties in current predictive tools lead current combustion-system developers to include significant margins of safety to ensure compliance with emissions regulations. For example, compression-ignition engines currently must be designed to meet emissions standards that are significantly tighter than the requirements to allow for uncertainties and variability, and this generally is done at the expense of reduced efficiency. Reducing the uncertainties would allow the margin of safety to be relaxed, thereby realizing a 30% to 50% gain in fuel economy while still meeting emissions standards.

Similarly, the compression ratio of modern spark-ignition engines is kept lower than theoretically necessary (thereby reducing efficiency) and the structure of the engine is over-designed (thereby increasing weight and cost) to minimize engine knock and to protect against the occasional occurrence of knock. These very conservative design practices could be relaxed if the uncertainty associated with knock prediction could be reduced, and efficiency would increase commensurately. Moreover, in the final installation of a spark-ignition engine for a production vehicle, any gains in efficiency that have been realized in controlled laboratory conditions are reduced because of the need to calibrate the engine to account for variability and uncertainty. These increments in efficiency could be regained with more predictive modeling tools.

PreSICE design tools can impact broader transportation engine design

The goal of off-highway transportation engine combustion systems is to provide a high fuel conversion efficiency, robust operation, wide operability, and low emissions, whether for heavy equipment, trains, planes, or ships. This sounds very similar to the goal of an internal combustion engine system for cars and trucks, and, in fact, many similarities do exist. For example, all systems must deliver, atomize, and evaporate liquid fuel prior to the combustion process. Therefore, each combustion architecture must deal with both the complexity of fuel preparation and the primary and secondary spray breakup processes. In addition, all combustion architectures rely on a good understanding of fuel–air mixing and chemistry as they strongly impact the emissions of NO_x, CO, UHC, and soot. As in the car and truck internal combustion engine industries, legislation continues to be introduced aimed at reducing emissions from off-highway engines.

Many of the software tools to be developed for car and truck internal combustion engines will be applicable to these other engines. Additional development will be required to ensure validation of predictive capability with the following considerations:

- A broader investigation of fuel injection techniques is needed; for example, aircraft engines often rely on air-assisted atomization techniques as opposed to pressure driven atomization.
- A broader examination of operating conditions is required, recognizing for example that the density ratios can be quite different between an aircraft engine and an internal combustion engine.
- The fuels considered need to be expanded to include Jet A fuel, commonly used in aircraft, and bunker fuel used in shipping, both of which have different volatility, density, and viscous properties relative to diesel and gasoline.

One of the largest contributors to uncertainty in combustion calculations and limitation to investigating novel combustion strategies and geometries is today’s spray models. Presently, practical spray models start at the fuel injector exit plane. The models are empirical in nature and optimized for pressure atomization. The combustion design process today requires that the combustion models be calibrated with data from a “similar” combustion system prior to launching a new combustion design. The largest unknowns in that process are the spray characteristics. The adjustments available in the spray model have a substantial impact on the ability of the combustion calculation to match the empirical data and create significant uncertainty in the combustion calculations. Furthermore, the models are not directly applicable to newer injection techniques under consideration, where fuel is injected at supercritical conditions or acoustic waves are used to break up the fuel at lower injection pressures, etc. In addition, the models do not account for injector geometry, cavitation of the liquid fuel during delivery, or the transient nature of injection events.

Delivering the capability defined in the spray focus area will address these gaps. Treatment of fuel delivery systems (internal flows) will create the capability to accurately predict boundary conditions for the fuel as it is delivered to the combustion chamber as a function of time. This advance will enable a significant improvement in the ability to predict the movement of the fuel during the combustion calculations. In addition, injectors can be designed to deliver spray characteristics that are desired by the combustion chamber; cavitation can be predicted and avoided as required to increase injector durability; coking in the injector can be avoided; and analysis of novel fuel injector/combustion concepts can be supported. Similarly, treatment of fuel preparation strategies (in-cylinder flow, mixing, and combustion) and in-cylinder fluid–wall interactions and heat transfer will provide the means to accurately predict the fuel distribution in the combustion chamber.

The limits of current physical models force substantial calibration of model coefficients before a combustion code can be used for a specific design problem, and the calibration is only valid over a relatively narrow range of operating conditions. Reducing or eliminating this calibration step alone would speed the development process significantly (up to 33%). Finally, the limits of current physical models translate to significant fractions of engine development time; today 33% to 50% must be spent on final engine calibration. The availability of predictive simulation tools would reduce overall engine development time and cost by 30% or more. These savings will both increase the competiveness of industry and provide better value to the consumer. Predictive simulation design tools for engines will thus enable 30% to 50% more efficient engines to be delivered more quickly to the market at competitive prices.

Conclusion

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Building on previous DOE workshops and research community strategy sessions considering improved engine combustion efficiency, the primary stakeholders in industry, academia, national laboratories and government came together at the PreSICE workshop on March 3, 2011. The workshop clearly identified and articulated two strategic focus areas that will accelerate innovation in engine design needed to meet national goals in transportation efficiency. Tremendous progress toward these goals can be made by enhancing engine fuel efficiency by 30% to 50%.

While workshop participants agreed such enhanced efficiency is achievable, they also agreed that dramatic increases in engine efficiency can only be reached by developing new design tools that fully leverage the computational simulation capabilities of the nation. These advanced capabilities will result in direct economic benefit through reduced time-to-market and reduced development costs. Dramatic increases in fuel efficiency will increase the nation’s energy security and simultaneously reduce greenhouse emissions. Advanced combustion research indicates that substantial improvements in efficiency are possible, but the processes are sensitive and require high levels of precision. In addition, long societal times scales are required to fully implement solutions and pressures from international competition are significant. Overcoming these issues will require greatly improved efficiencies in the research, design, and development processes.

Modeling and simulation technology is on the verge of providing the essential tools that can be used to achieve much higher fuel economy and a greatly improved development timescale. The simulations must be supported by basic research to improve fundamental understanding and provide essential data for model improvements. Participants at the PreSICE workshop identified two strategic focus areas that will enable the desired simulation capability: fuel sprays and stochastic processes.

Fuel sprays will set the initial conditions for combustion in essentially all future transportation engines, and yet today sprays designers primarily use empirical methods that limit the efficiency achievable. Three primary spray topics were identified as focus areas in the workshop:

1. The fuel delivery system, which includes fuel manifolds and injectors,
2. The fuel–air mixing and preparation in the combustion chamber of the engine, and
3. The heat transfer and fluid interaction with cylinder walls.

All of these areas require improved basic understanding, high-fidelity model development, and rigorous model validation. These advances will greatly reduce the uncertainties in current models and improve the understanding of sprays and fuel–air mixture preparation that limit the investigation and development of advanced combustion technologies.

Current understanding and modeling capability of stochastic processes in engines remains limited and prevents designers from achieving significantly higher fuel economy. To improve this situation, the workshop participants identified three focus areas for stochastic processes:

1. Improve fundamental understanding that will help to establish and characterize the physical causes of stochastic events,
2. Develop physics-based simulation models that are accurate and sensitive enough to capture performance-limiting variability, and
3. Quantify and manage uncertainty in model parameters and boundary conditions.

Improved models and understanding in these areas will allow designers to develop engines with reduced design margins and that operate reliably in more efficient regimes.

The two strategic focus areas have distinctive characteristics but are inherently coupled. Coordinated activities in basic experiments, fundamental simulations, and engineering-level model development and validation can be used to successfully address all of the topics identified in the PreSICE workshop. The outcome will be:

1. New and deeper understanding of the relevant fundamental physical and chemical processes in advanced combustion technologies,
2. The implementation of this understanding into models and simulation tools appropriate for both exploration and design, and
3. Sufficient validation with uncertainty quantification to provide confidence in the simulation results.

These outcomes will provide the design tools for industry to reduce development time by up to 30% and improve engine efficiencies by up to 30% to 50%. The improved efficiencies applied to the national mix of transportation applications have the potential to save over 5 million barrels of oil per day, a current cost savings of $500 million per day.

Appendix I: Workshop Attendees

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Name	Affiliation
John Abraham	Purdue University
Dennis Assanis	University of Michigan
Tom Avedisian	Cornell University
Fritz Bedford	ANSYS
Bill Brinkman	DOE SC
David Carrington	Los Alamos National Laboratory
Michael Cassasa	DOE SC/BES
Steve Ciatti	Argonne National Laboratory
Kathryn Clay	Auto Alliance
Chris Cowland	Chrysler
John Deur	Cummins
Anne Dord	General Electric
Derek Dunn-Rankin	University of California, Irvine
Mike Drake	General Motors
Wayne Eckerle	Cummins
Dan Flowers	Lawrence Livermore National Laboratory
Caroline Genzale	Georgia Tech University
Dan Haworth	Pennsylvania State University
Bob Gemmer	DOE EERE
Ron Graves	Oak Ridge National Laboratory
Richard Johns	CDAdapco
Steve Koonin	Under Secretary for Science
Tang-Wei Kuo	General Motors
Stephen Klippenstein	Argonne National Laboratory
Randall Laviolette	ASCR
Ed Law	Princeton University
Jerry Lee	United Technologies Research Center
Stephen Leone	Lawrence Berkeley National Laboratory
Cynthia Lin	Office of the Under Secretary for Science
Tom McCarthy	Ford
Andy McIlroy	Sandia National Laboratories
Paul Miles	Sandia National Laboratories
Ellen Meeks	Reaction Design
Amy Mullin	University of Maryland
George Muntean	Pacific Northwest National Laboratory
Joe Oefelein	Sandia National Laboratories
Melissa Patterson	Sandia National Laboratories
Mark Pederson	SC/BES

Name	Affiliation
Walt Polansky	SC/ASCR
Eric Rohlfing	DOE SC/BES
Chris Rutland	University of Wisconsin
Ramanan Sankaran	Oak Ridge National Laboratory
Peter Schihl	U.S. Army/TARDAC
Peter Senecal	Convergent Science
Gurpreet Singh	DOE EERE/VT
Volker Sick	University of Michigan
Wade Sisk	DOE SC/BES
Ceren Susut-Bennett	DOE SC/ASCR
Craig Taatjes	Sandia National Laboratories
Angela Violi	University of Michigan
Dave Walker	General Electric
Charlie Westbrook	Lawrence Livermore National Laboratory
Margaret Wooldridge	University of Michigan
James Yi	Ford
Hua-Gen Yu	Brookhaven National Laboratory

Appendix II: Workshop Agenda

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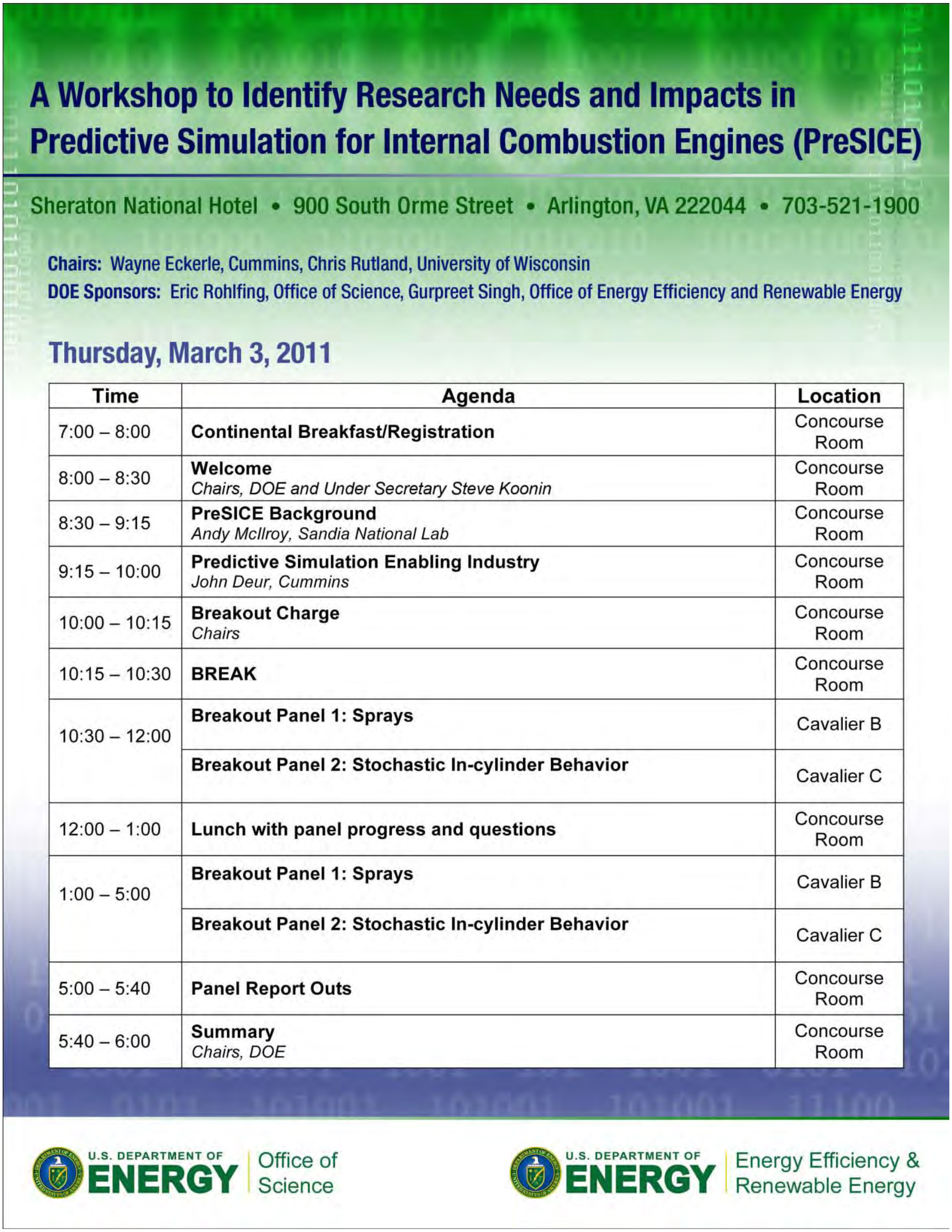

A Workshop to Identify Research Needs and Impacts in Predictive Simulation for Internal Combustion Engines (PreSICE)

Sheraton National Hotel • 900 South Orme Street • Arlington, VA 222044 • 703-521-1900

Chairs: Wayne Eckerle, Cummins, Chris Rutland, University of Wisconsin

DOE Sponsors: Eric Rohlfing, Office of Science, Gurpreet Singh, Office of Energy Efficiency and Renewable Energy

Thursday, March 3, 2011

Time	Agenda	Location
7:00 – 8:00	**Continental Breakfast/Registration**	Concourse Room
8:00 – 8:30	**Welcome** *Chairs, DOE and Under Secretary Steve Koonin*	Concourse Room
8:30 – 9:15	**PreSICE Background** *Andy McIlroy, Sandia National Lab*	Concourse Room
9:15 – 10:00	**Predictive Simulation Enabling Industry** *John Deur, Cummins*	Concourse Room
10:00 – 10:15	**Breakout Charge** *Chairs*	Concourse Room
10:15 – 10:30	**BREAK**	Concourse Room
10:30 – 12:00	**Breakout Panel 1: Sprays**	Cavalier B
	Breakout Panel 2: Stochastic In-cylinder Behavior	Cavalier C
12:00 – 1:00	**Lunch with panel progress and questions**	Concourse Room
1:00 – 5:00	**Breakout Panel 1: Sprays**	Cavalier B
	Breakout Panel 2: Stochastic In-cylinder Behavior	Cavalier C
5:00 – 5:40	**Panel Report Outs**	Concourse Room
5:40 – 6:00	**Summary** *Chairs, DOE*	Concourse Room

U.S. DEPARTMENT OF ENERGY | Office of Science

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

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Sponsored by the Office of Basic Energy Sciences, Office of Science and the Vehicle Technologies Program, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy

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