Simulating Real-World Combustion Devices

Combustion of fossil fuel is central to the U.S. economy, accounting for 85 percent of the energy consumed in the United States each year. Combustion of fossil fuels provides a level of comfort and mobility for U.S. citizens that is unrivaled in the world. At the global level, fossil fuels will continue to be the primary source of energy required for economic growth. Despite continuing investments in alternative energy sources, the importance of fossil fuels, as they relate to the economy and quality of life in the United States and abroad, is unlikely to change in the foreseeable future.

Although the cost of fossil fuels was a staggering $334 billion in 1996, combustion efficiency has not been a major issue in the United States since the oil crises of the mid 1970s and early 1980s when U.S. dependence on foreign sources of crude oil led to major economic and societal dislocations. Today, fossil fuels are inexpensive and the supply remains stable despite continued dependence on foreign sources of oil. Combustion efficiency has returned as an issue of national concern, not because of our dependence on foreign oil, but in response to recent changes in environmental mandates. A critical component of President Clinton's comprehensive environmental framework, his climate change proposal, is aimed at reduction of greenhouse emissions to 1990 levels by 2008-2012, with reductions below 1990 levels in the five-year period that follows. These goals coupled with consumer demands will have a profound impact on the design and operation of the combustion systems of the future.

Combustion of fossil fuels is responsible for nearly all of the anthropogenic emissions of nitrogen oxides (NOx), carbon monoxide (CO), soot, aerosols, and other chemical species that are harmful or are suspected to be harmful to human health and the environment. To meet the goals set forth by current U.S. policy, a balanced approach that considers efficiency, cost, and emission levels must be developed. Radically new engine designs are the only hope for meeting the near-zero NOx and particulate emissions commitments set forth by U.S. public interest and proposed for implementation by 2012. *Dramatic advances in the computational modeling and simulation of complex real-world systems, enabled by continuing advances in high-performance computing, offer an opportunity to revolutionize the design and performance of current combustion systems*.

Combustion simulation aims to provide new, fundamental knowledge about combustion processes, emphasizing those combustion systems that will have the greatest impact on the economy and the environment in the United States. These include both gasoline- and diesel-fueled internal combustion engines; large-scale boilers and turbines (used for production of electricity); industrial combustion devices (used primarily for process heat), including boilers and furnaces and turbines.

Other Applications

Advances in combustion simulation, through the development of computational tools to model complex processes, will be broadly applicable to other processes that involve turbulent, chemically reacting flows. These processes range from chemical, glass, and metal manufacturing, microelectronics fabrication, to such health-related areas as blood flow and chemistry.

Combustion devices are complex systems that include the fuel and exhaust streams, the combustion device itself, and all processes that occur in the combustion chamber. The development of predictive computational models for realistic combustion devices is a challenging task. Combustion modeling requires the integration of a broad array of computational physical and chemical submodels into a comprehensive model of the physical combustion device itself. Combustion systems involve three-dimensional, time-dependent, turbulent flows in complex physical configurations, and, in the case of internal combustion engines or turbines, moving components. Many of these flows involve multiple fluids with liquid droplets and solid particles that are transported through the gas phase. Against this fluid-dynamical backdrop, chemical reactions occur that determine the energy production in the system, as well as the emissions that are produced. For complex fuels, the chemistry involves hundreds to thousands of chemical species participating in thousands of reactions.

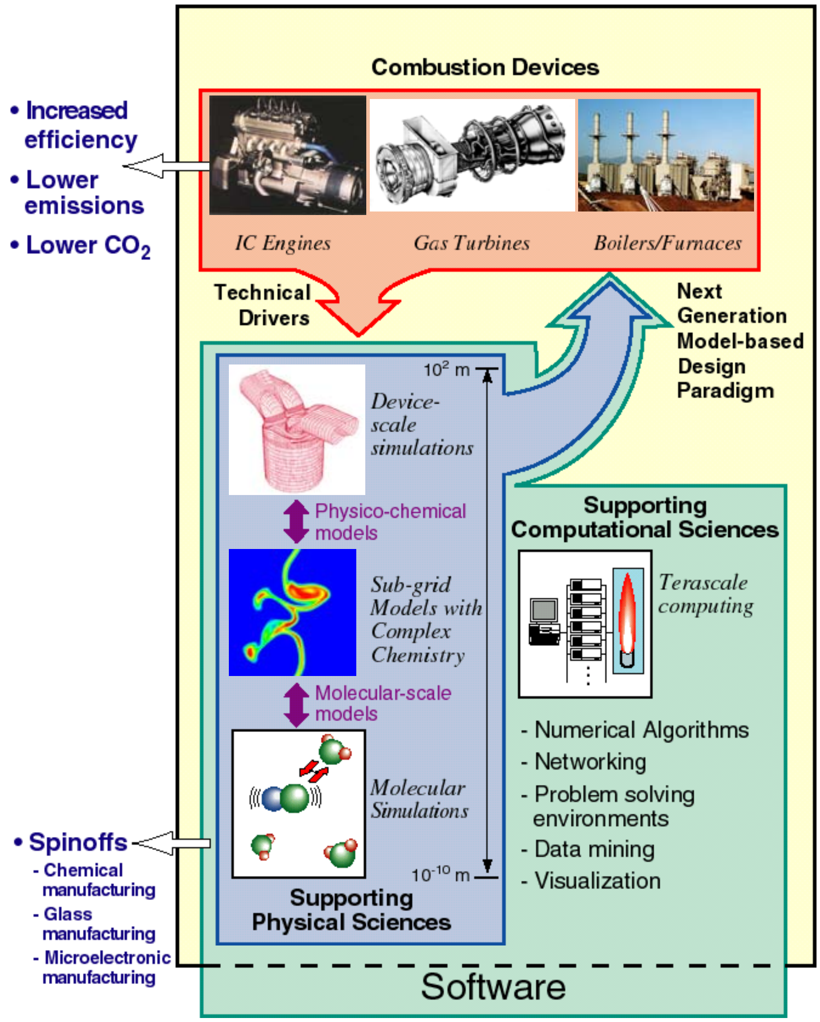
In addition to the above, the phenomena that influence combustion span a wide range of scales in space and time. The spatial scale extends from the dimensions of molecules, billionths of a meter, where chemical reactions occur up to the scale of the combustion device itself, which is measured in meters. Chemical reactions occur in billionths or even trillionths of a second while the warm-up time for an internal combustion engine is measured in minutes. The computational task of addressing this range of time and length scales is at the heart of the scientific challenges facing the development of predictive models.

Until now, the limited capabilities of available computational resources, has led to the use of over-approximation in the simulation of combustion processes. For example, multi-cycle simulations of internal combustion engines are required to predict the transient phenomena that are responsible for the emissions that occur during the first few minutes of engine operation. Yet today, single-cycle calculations with relatively crude submodels containing minimal or no chemistry represent the state-of-the-art.

With a focused effort involving

- multidisciplinary teams of theoretical and computational physicists and chemists working closely with computer scientists and applied mathematicians and
- terascale computer systems operating at over ten trillion arithmetic operations per second,

Combustion Simulation & Modeling



a new generation of computational models for real-world combustion devices will be realized that overcome today's limitations. These tools will lead, *for the first time*, to high-fidelity, fully predictive simulation of complete combustion devices.

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