Chemically reacting flows feature prominently in the majority of energy conversion and propulsion systems. Reacting flow governs their efficiency; the formation of hazardous pollutants and greenhouse gases; the system reliability; size; power density; etc. These systems are of paramount importance to national security, health, economic competitiveness, and environmental quality. At the current worldwide power consumption of 14 terawatt, with 85% fossil fuel combustion based, and the projected 3X increase over the next 50 years, the economic and environmental consequences are staggering. There is an immediate need to deliver high performance power systems for a spectrum of applications ranging from handheld devices, wearable electronics, at the sub-watt level, to long range high speed transportation systems, and very large-scale power plants that satisfy the insatiable and rapidly growing need for energy around the globe. Additionally, reacting flows of similar nature and complexity have become increasingly important in manufacturing processes and material synthesis, where they are applied to transform material properties and create new materials; fabricate new macro, micro and nano structures for a wide range of applications including semiconductors and optoelectronics.

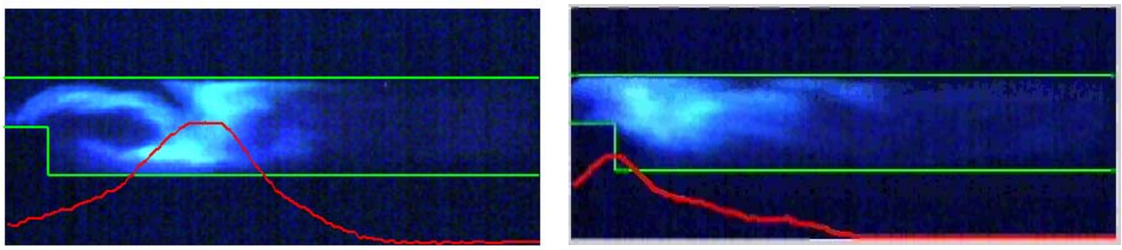
The field of chemically reacting flows encompasses a wide range of processes, including combustion; liquid and gaseous fuel reforming and synthesis; solid fuel gasification and separation of lighter components; hydrogen production, from hydrocarbon fuels and thermonuclear energy, efficient, compact and fast hydrogen storage and retrieval; fuel cells and batteries for direct conversion; micro and nanoscale material synthesis; etc. In these processes, the interactions between thermochemistry, electrochemistry, molecular and charged particle transport, flow of complex fluids, turbulence, electromagnetic waves, adsorption and desorption and other interfacial phenomena lead to the conversion of chemical bond energy, thermal and electromagnetic wave energy to mechanical energy and electricity, and/or the transformation of the molecular structure of fuels and materials. The drive to design small scale power for portable electronics, and wearable electronics for biological functions; ultra clean energy systems; zero emission power systems with greenhouse sequestration, depends critically of understanding and predicting multiscale phenomena over a wide range of conditions in different environments.

Chemically reacting flows are inherently multiphysics problems that can include acoustics and other long and short wavelength electromagnetic waves, convective and molecular level transport, homogeneous and heterogeneous chemical and electrochemical kinetics, multiphase phenomena, and flow in catalytic microchannels. In some systems and under some conditions, the continuum approximation is valid and the reactive Navier-Stokes equations are used, supplemented with constitutive, thermodynamic and kinetic equations that describe material properties, state relations and chemical transformations. Even within the continuum approximation, the significant scales in a typical chemically reacting flow system span over 6 decades in space and 9 decades in time; with dependent variables that vary over a similar range. In other problems, in which solid or liquid particulates are either introduced or form as a byproducts of the chemical reaction, e.g., soot, the range of scales increase by two decades to capture the interactions. In yet a more complex class, where surface and microchannel catalytic interactions play an important role, further reduction of the smallest scales are encountered due to the lack of high fidelity constitutive transport models near the surfaces that forces one to consider a heterogeneous molecular scale-continuum scale formulation. A similar requirement is encountered in material synthesis, where highly localized combustion processes are used at the micro to nano scale, while traversing macro dimensions, in complex material structure.

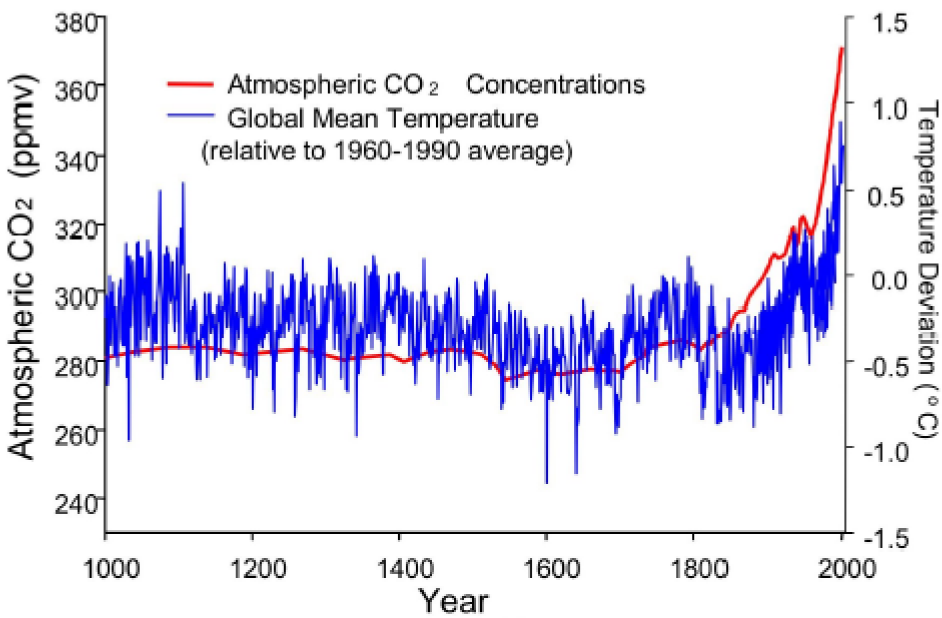
Novel power and propulsion systems have the potential to achieve 2-3X efficiency improvement, thus reducing the nation's dependence on foreign oil supplies and limiting the formation of greenhouse gases; and reach near zero emissions of toxic pollutants and minimal greenhouse gases, while using unconventional fuels. Examples of such energy systems and processes include lean stable combustion in continuous or intermittent combustion engines, ultra lean combustion in catalytic microchannels, low temperature, short time scale conversion in nanotubes for reforming and hydrogen storage, concurrent reforming and direct energy conversion in microfuel cells that utilize conventional fuels to produce electricity and hydrogen; extremely fast burning in high speed compact channels; reversible fuel cell- electrolyzer units, propulsion systems for high speed water propulsion, actively controlled power and propulsion systems that adopt to changes in their environment, hybrid systems that optimize the operation of the overall system by etc. Many of these systems must be developed to enable transition to a hydrogen-based economy.

Design of these systems require analysis tools that capture the characteristics of reacting flow processes beyond what is currently known and understood; where all current phenomenological models are known to fail; and where current computational techniques can not produce reliable results within acceptable turn around time. Achieving these goals require high fidelity physical models, some of which are more likely to be known at the microscale only, and accurate computational algorithms that couple heterogeneous domains that span continuum to the atomistic scales. High fidelity simulations obtained using these tools must respond faithfully to small changes in the design; operating condition; fuel chemistry or other material properties in order to be useful and gain acceptance in engineering. These simulations must also be optimized to run within reasonable turn around times to enable parametric studies and produce optimal designs that can meet more requirements that can be achieved today. The levels of accuracy of the computational results must reach the same levels as those imposed on power systems that cannot emit more than few particles per millions of nitric oxide and three orders of magnitudes less in solid particulates before it is licensed for operation.

The design and operation of efficient, clean and reliable energy and propulsion systems, from the sub-watt to the terawatt levels, can be fundamentally transformed if computationally based accurate and efficient simulation tools become available. These tools will have to address/exploit the multiscale nature of reacting flow processes, accurately and efficiently, and achieve the level of fidelity required to meet the stringent performance demands of energy systems.



High-speed images of a lean burn combustor showing the flame contour in light blue, and the heat release rate distribution, depicted a redline. On the left hand side, the combustion process is unstable, and the flame oscillates at a frequency of 38.5 hz. On the right hand side, a hydrogen-air transverse jet is injected near the step to stabilize the flame. Hydrogen concentration is less than 2% of the total fuel concentration.



Increased CO2 Emissions Causing a Rise in Atmospheric CO2 Associated with a Rise in Global Temperature (Sources: CO2 data from Ethridge et al. 2001, Keeling and Whorf 2002; temperature data from Jones et al. 1998, Peterson and Vose 1997) From BES Workshop on Basic Research Needs for the Hydrogen Economy

Air pollution from emissions -- Washington, DC, November 2003