

Autoignition and Control of 'Flameless' Combustion

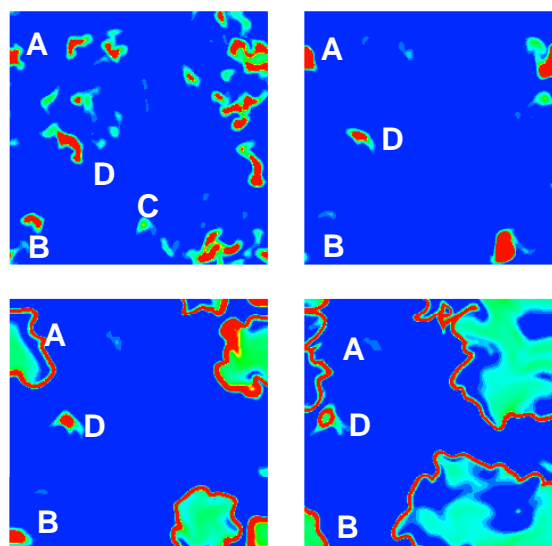
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Autoignition is the process that lights a combustible mixture by the mere application of heat, but without a flame or spark. For example, autoignition lights the combustion process every time a diesel truck engine cylinder fires. Autoignition also limits the efficiency of most automobile engines, and produces undesirable 'flashback' in low-emission gas turbine combustors that are used to generate electricity. A major scientific question is; How does autoignition progress in fluctuating and incompletely mixed gases, and how we might control the process?

An even more important motivation for this scientific question is a very interesting idea for novel high efficiency, low emission combustion technologies. Experiments show autoignition allows us to initiate combustion in a gas mixture that will not burn otherwise. That is, it will not burn in the usual mode where fuel is consumed in a thin high-temperature sheet of flame. An important application of such 'flameless' combustion is inside the chamber of a revolutionary new, efficient internal combustion engine with extremely low emissions. The catch is that such high-efficiency, low emission power plants (termed Homogeneous Charge, Compression Ignition, or HCCI engines) are useless for cars and trucks because we have not yet learned how to control 'flameless' combustion! Thus, auto manufacturers cannot yet produce the response in this type of engine that we all expect when we jump into our cars to run down to the market for groceries. The successful application of HCCI engine technology to light-duty vehicles would save 25 to 30 billion gallons of gasoline each year, or 16% of US imported crude oil. Application to heavy-duty vehicles would dramatically reduce NO_x emissions (heavy-duty diesels contribute about one-half of all highway NO_x). A key hope in this community is that a better fundamental understanding and resulting control of autoignition will enable a long-sought after breakthrough for this combustion concept.

Our present understanding of autoignition is primarily from experimental data and simulations limited to zero or one-dimensional studies. (Such as in shock tubes, rapid compression machines, and, recently, in steady laminar one-dimensional experiments and simulations.) Most of this work assumes perfectly mixed gases with no spatial variations. However, in reality, autoignition in fluctuating environments is a highly transient chemical process (time scales of less than 1 millisecond) involving many short-lived molecular species within a three-dimensional spatial structure that dynamically evolves. It is the details of this



Islands of hydroperoxy (HO_2), an early indicator of autoignition, are shown forming in 2-D simulations of a fluctuating hydrogen-air mixture (in time from top left to lower right). Note that kernel A grows most rapidly, D most slowly, and that C is extinguished by the fluctuations.

transient chemical and dynamical structure that we do not understand. The complex dynamical nature of such autoignition processes cannot be captured with current experiments and simulations, and the required information is well beyond what we can hope to measure with sophisticated laser-based experiments. But terascale computer simulations offer the opportunity to study this complex phenomena in great detail giving us the keys to innovative 'flameless' combustion technologies as well as other important ignition phenomena.

In the past year we have been able to perform 2-dimensional pilot simulations of autoignition in mixtures of hydrogen and air. From these Direct Numerical Simulations (DNS) we have identified new chemical pathways for ignition to proceed in such fluctuating environments, and have proposed a new approach to describing transient autoignition in terms of relevant flow and thermochemical parameters. The simulations show that autoignition is initiated in discrete kernels or structures that evolve differently, depending strongly upon the exact local environment in which they find themselves as shown in the Figure. But this work has only provided a glimpse into the real problem. Turbulent fluctuations as well as the autoignition kernels are inherently 3-dimensional, and more complex fossil fuels will produce new time-dependent behaviors that must be studied in a full range of fluctuating environments to gain scientific insight to develop and quantitatively validate predictive models.

The direct numerical simulations shown in the figure are limited by currently available computational resources to two dimensions and either to simple flow processes, or simple chemistry. This pilot study required about 2×10^{16} math operations and was carried out with the Sandia S3D computer code that makes effective use of over 1000 processors. It required ~300,000 node-hrs for three runs having different sets of initial parameters on the NERSC IBM SP3 (4 Tflops) machine. Running on 256 processors, it took about 2-4 weeks turnaround time per run (including time waiting in batch queues.) The volume of data generated for this work (3 runs at 2D, hydrogen/air ignition, 8 reactive species, 1.8 million grid points) is about 244GB.

The actual scientific requirement is for a series of 3D runs to study n-heptane (a surrogate for more complex hydrocarbon fuels) autoignition. The increased chemical complexity (44 species) and size ($\sim 10^8$ grid points) will require $\sim 3 \times 10^{18}$ math operations and would produce up to 100 TB of data to analyze. This study would require about 10 hrs at a sustained computational rate of 100 Teraflops or 50 hrs at a sustained 20 Teraflops. With increased code efficiency (S3D currently runs at 7% of peak efficiency at NERSC) and/or more optimal computer architectures, such a project could be carried out on a 40-50 TeraFlops machine on reasonable time scales.

This simulation would provide the first realistic simulation of a moderately complex, but realistic, autoignition process revealing its topologies and propagation dynamics. The data would provide a fundamental understanding of the effect of mixing on the dynamics of autoignition, and would ultimately stimulate new strategies for mixing fuel and air to achieve the desired operating flexibility and control while maintaining high efficiency and low emissions.

This research also would help unveil the complex fundamental relationships between useful energy output and undesired emissions (almost exclusively NO_x and Soot) in combustion devices, giving the Nation a stronger basis for decisions on policy and choices among programs such as PNGV, fuel cell development, homogeneous charge compression ignition engines, or increased CAFE standards for cars and trucks.