



U.S. DEPARTMENT OF
ENERGY

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SciDAC
Scientific Discovery through Advanced Computing

Understanding Pre-Mixed Turbulent Combustion

Peer-Timo Bremer¹, Gunther Weber², Valerio Pascucci³, Marc Day², John B. Bell²

¹Lawrence Livermore National Laboratory; ²Lawrence Berkeley National Laboratory; ³University of Utah

Summary

There have been significant recent efforts to better understand the nature of turbulent combustion in order to guide the design of new fuel-efficient, low-emission engines and turbines. However, adding turbulence to the already complicated combustion process results in seemingly chaotic intricate reactions that are difficult to analyze. Scientists from the SciDAC Visualization and Analytics Center for Enabling Technology (VACET) have developed a suite of general purpose data analysis tools based on Morse theory that can reliably process large, time-dependent scientific data sets regardless of their underlying complexity. Using Morse theory, we compute hierarchical topological graphs that encode complete families of structural segmentations. Despite being orders of magnitude smaller than the original data, these graphs enable data exploration at multiple spatiotemporal scales and within a wide range of parameters. In particular, the hierarchy supports extensive parameter studies without the need for potentially expensive re-processing of the original data. The resulting statistics enable scientists to select appropriate parameters and provide insight into the impact of the choice of parameters on the results. These new methods enable a new form of scientific understanding: the ability to quantitatively correlate the turbulence of the burning process with the distribution of burning regions properly segmented and selected. Our analysis shows a new, counter-intuitive result: stronger turbulence leads to larger cell structures, which burn more intensely than expected.

Understanding combustion processes over a broad range of operational regimes is of great interest for a variety of applications like engine or power plant design. To this end, there has been considerable recent interest in the development of premixed burners capable of stably burning ultra-lean hydrogen-air fuel mixtures. Such burners could, for example, be used as one component of a clean-coal power plant utilizing hydrogen extracted from coal gasification. Lean premixed systems are subject to a variety of hydrodynamic and combustion instabilities that render practical flame stabilization, and traditional approaches to flame analysis, extremely difficult. The flames burn in a cellular mode that is highly non-uniform, time-dependent, and difficult to characterize.

To study the combustion process at different levels of turbulence, scientists at the Lawrence Berkeley National Laboratory performed numerical simulations of lean premixed hydrogen flames in three different turbulence configurations: no turbulence, weak turbulence, and strong turbulence. Our analysis characterizes

the burning behavior in these systems by the number and size of burning cells. We represent flames as isotherms of constant temperature. On each flame surface, thresholds on the local fuel consumption divide the surfaces into burning cells separated by non-burning regions.

To gain new insights into the combustion process, scientists are interested in two types of analysis: time-aggregate statistics and detailed analysis of cell evolution. Comprehensive statistics on the number and area of burning cells aggregated over time provide important information about quantitative and qualitative differences between flames under different levels of turbulence. A tracking graph representing the evolution of cells over time describes the local cell dynamics in detail and enables an in depth study of all temporal events, such as cell births, deaths, merges, and splits. Coupling the tracking graph to an interactive visualization of the segmented flame surfaces illustrates each event and is an important tool to verify and validate the parameter selection.



VACET

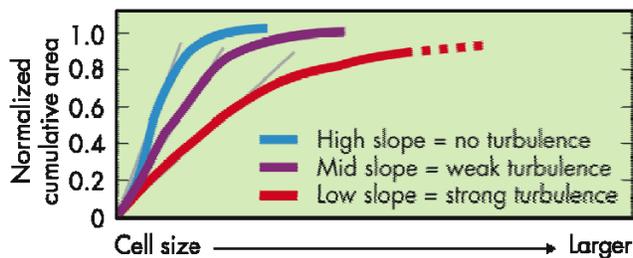
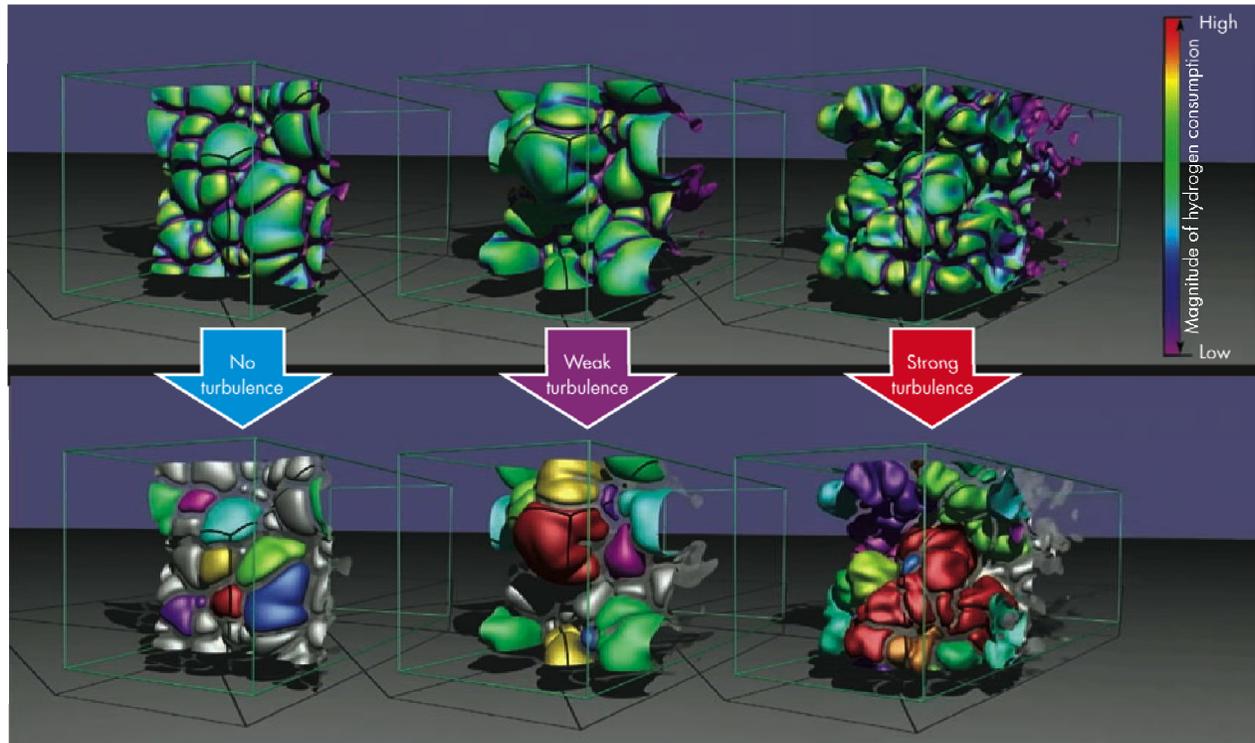


Figure 1. The top 3D diagrams show flame surfaces of a lean premixed hydrogen flame at different levels of turbulence colored by the local fuel consumption. In the bottom 3D diagrams a small set of burning cells are randomly colored to show the irregularity of the more turbulent cells. In the graph, the corresponding cumulative density function of cell area distributions show that more turbulence creates larger cells with a wider distribution of normalized surface areas indicating a more intense burning process.

However, no unique correct threshold exists, so a primary goal is to determine and verify the choice of parameters. Using the parallel computing resources at NERC we extract the isotherms for each time-step of the simulation and compute merge trees of the fuel-consumption function defined on the isotherms. Each tree encodes the cell configurations for all possible thresholds, and we augment the trees by storing cell areas as a function of the threshold along their corresponding branches. We use the augmented trees to perform extensive parameter studies, which determined a viable threshold and demonstrated the consistency of the results using varying parameters. Once we determine a threshold, we track the corresponding burning cells through time and create a tracking graph that encodes their temporal evolution. Our methods allow, for the first time, a quantitative analysis of the cellular burning structures and yield important scientific insights: Although it seems counterintuitive, higher turbulence levels lead to larger cell structures, which also burn more intensely than predicted by simple theories of flame propagation. These results suggest that premixed hydrogen flames could be stabilized at much leaner conditions than previously believed.

Recent Publications

M. Day, J. Bell, P.-T. Bremer, V. Pascucci, V. Beckner, M. Lijewski, "Turbulence effects on cellular burning structures in lean premixed hydrogen flames", *Combustion and Flame*, in press.

G. Weber, P.-T. Bremer, V. Pascucci, M. Day, and J. Bell, "Feature Tracking Using Reeb Graphs", in *Proc. 3rd TopoInVis Workshop*, to appear.

For further information on this subject contact:

Name: Peer-Timo Bremer.
 Organization: Lawrence Livermore National Laboratory.
 Email: bremer5@llnl.gov
 Phone: (925) 454-0465

Note: This work was funded in part by the SciDAC2 Visualization and Analytics Center for Enabling Technologies and has been performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.