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Computational combustion

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Abstract

Progress in the field of computational combustion over the past 50 years is reviewed. Particular attention is given to those classes of models that are common to most system modeling efforts, including fluid dynamics, chemical kinetics, liquid sprays, and turbulent flame models. The developments in combustion modeling are placed into the time-dependent context of the accompanying exponential growth in computer capabilities and Moore's law. Superimposed on this steady growth, the occasional sudden advances in modeling capabilities are identified, and their impacts are discussed. Integration of submodels into system models for spark ignition, diesel and homogeneous charge, compression ignition engines, surface and catalytic combustion, pulse combustion, and detonations are described. Finally, the current state of combustion modeling is illustrated by descriptions of a very large jet lifted 3D turbulent hydrogen flame with direct numerical simulation and 3D large eddy simulations of practical gas burner combustion devices.
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1. Introduction

As the Combustion Institute celebrates its 50th anniversary, it is an interesting coincidence that the science of computer simulation and modeling is also approximately 50 years old. Beginning as a technical curiosity with minor impact on scientific research, computer modeling has grown rapidly to play a major role in virtually every field of science and engineering. In particular, computer modeling is now an essential part of combustion research; at the larger scale, enormous computer simulations are assisting in design and optimization of internal combustion engines, solid fuel rocket motors, industrial burners and furnaces, and gas turbine combustors, using massively parallel supercomputers. At the smaller scale, computer simulations are ubiquitous in everyday combustion life, being used to control operation of individual laboratory experiments, fit spectra in basic science studies, and a multitude of other research and routine applications.

Of course, the electronic computer is not the only modern feature of combustion science. In fact, most of the tools we use today have appeared and become essential during the past 50 years. It is almost impossible today to imagine a research project without the laser, the gas

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chromatograph or mass spectrometer, and many other tools, in addition to the computer. And each of these tools has grown rapidly in terms of capabilities and importance, although the growth of the computer as a tool has outstripped them all. All of them are indicative of the rapid pace of technological growth, and we must assume that future growth will be at least as rapid and profound. We should continually ask ourselves if we are realizing comparable growth in our understanding of and ability to control the combustion processes that are so much a part of our lives. As we will hope to describe in this paper, computer simulations have certainly added a great deal of understanding, providing fundamental answers to many long-standing questions.

Computational combustion is an enormous topic, with many of the different aspects deserving and receiving reviews by themselves. We are attempting to provide an unusual sort of overview, highlighting those areas in which computer simulations have made an important difference in the way we do research, and emphasizing some of the computational contributions that have provided unique and important insights into the nature of combustion itself. These range from cases in which modeling solved long-standing puzzles or problems, to cases in which modeling changed the views of the entire combustion community. We highlight the case of HCCI combustion, where the existence of a mature simulation capability has revolutionized the overall research plan for an industry; the HCCI may or may not make a significant impact on power production, but we emphasize it because it illustrates the nature of the research team of the present and future, and the complete integration of computer modeling into research and development. We finish by taking the pulse of the near future in scientific computing to see what is about to become possible in terms of addressing difficult problems that have never been solved, simply because of their size and complexity. Combustion is one of many disciplines imbedded in a scientific world where the power of the computer is driving much of our progress, and we want to provide a glimpse of the next generation of problems that will be enabled just by continued growth in computer capacity.

This review is necessarily unbalanced; for example, we focus on modeling of laminar premixed flames and devote no space to laminar diffusion flames. We also discuss models of internal combustion engines but omit gas turbines and furnaces. The inclusions and exclusions reflect the strengths and weaknesses in the experiences of the authors, and they are also motivated by the limited space and time available to us. However, we have tried to include those areas in which computer modeling has grown and then made significant technical advances. In some cases, our choices were simplified by the existence of a recent expert review in some area that we could cite for those interested in further information. Our brief comments on soot modeling and modeling based on asymptotic analysis may be excused because we have assumed they will be discussed at length in one or more of the other review papers in this conference.

1.1. Background

Although computer modeling could not exist before the development of the computer, many essential tools were already in place before the arrival of the ENIAC and UNIVAC in 1952–1956. A considerable literature dealing with finite difference methods of solving differential equations had been developed, beginning with the paper of Courant et al. [1]. The solution techniques of Gaussian elimination for solution of simultaneous linear equations and Runge–Kutta methods for solving ordinary differential equations were also established before the arrival of the electronic computer [2]. There was also an enormous literature of careful, insightful experimental data for laminar flames, chemical kinetics, radiation transport, detonations, and many other problems; much of these experimental data and the technical insights based on these experiments were used in developing early numerical combustion models, and much of the same data are still waiting for computational combustion analysis.

The key person in the development of the first computers was John von Neumann, whose experience with transport and reactive flow problems led him to propose a concerted development effort following the end of the Second World War to produce an electronic computing machine, which was built at Princeton's Institute for Advanced Studies between 1946 and 1952. Ever since, scientific computing has been a discipline where researchers specialize in formulating problems that they know they cannot yet solve, although they know that the time will come when computer capabilities will catch up with their needs; of course, by the time they can actually complete that calculation, they will have again set their sights much higher, to another problem that cannot yet be solved. Scientific computing invented its own term for such problems, "Grand Challenges." At Supercomputing 88 [3], 16 years ago, the problems identified as unsolvable but important included aerodynamic flows over vehicles and through engines, and in-cylinder combustion flowfields, in addition to problems in many other fields, including the computing required to complete the human genome; in 2004, many of those problems are well on their way to solution, and people are formulating the next generation of Grand Challenge problems that cannot even be attempted today.