

MANIFOLD METHODS FOR METHANE COMBUSTION

1 August 1994 to 31 August 1996
FINAL REPORT

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**EXECUTIVE SUMMARY
AGTSR
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Project Title: Manifold Methods for Methane Combustion
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STATUS/ACCOMPLISHMENTS FOR THE REPORTING PERIOD

The overall objective of the project was to develop a computationally simple and efficient way to treat methane combustion chemistry. The method is sufficiently accurate to represent the detailed chemistry of interest, and yet efficient enough to be incorporated in turbulent combustion models such as PDF methods.

The end product is of direct usefulness; namely a methodology for efficiently computing methane combustion. The individual tasks along the way involved solving problems in the areas of applied mathematics and computer science.

1 Background

The overall picture is illustrated in Figure 1. In general, a problem in turbulent combustion is defined by the boundary conditions and the properties of fuel and oxidant (i.e., CH_4 and air). The turbulent combustion model we have in mind is a PDF method. In this case, for each of 10^5 (say) particles, on each of 10^3 (say), time steps, we need the simplified chemistry algorithm to answer the following question: Given the thermochemical composition of a particle at time t —denoted by $\phi(t)$ —what is the increment in the composition $\Delta\phi$ due to reaction over a specified time step Δt ? [Note: $\Delta\phi \equiv \phi(t + \Delta t) - \phi(t)$.]

We assume that an adequate detailed mechanism is available, giving the reaction rates $\mathbf{S}(\phi)$ as functions of the composition. Then, the increments can be obtained by direct numerical integration of the reaction equation

$$\frac{d\phi}{dt} = \mathbf{S}(\phi).$$

But this is prohibitively expensive computationally; and the objective of the project was to develop an alternative that is computationally much more efficient.

An alternative is to tabulate $\Delta\phi$. That is, in a pre-processing stage, Eq. (1) is integrated to obtain $\Delta\phi$ for particular values of ϕ , called tabulation points. Then in the turbulent combustion computation, an approximate value of $\Delta\phi$ is recovered by interpolation from the table. Unfortunately, this method (literally implemented) is also infeasible because of the high dimensionality of the composition space. That is, if there are $D \approx 20$, say, chemical species in the reaction mechanism, then ϕ can be considered as a point in the D -dimensional composition space. If just 10 tabulation points are used in each direction, then the total number, i.e., 10^D , is clearly prohibitively large.

More details about this algorithm and its use are provided in the report.

2 Approach

The approach we have taken uses a number of observation and techniques to make the tabulation method feasible. The first observation is that compositions ϕ that actually arise in turbulent combustion are very close to intrinsic low-dimensional manifolds (ILDm). That is, rather than filling the entire 20-dimensional space, compositions that occur lie close to three or four-dimensional surfaces. The second observation is that, for a given turbulent reactive flow, only a small fraction of the ILDM may be accessed, although the accessed region is difficult to determine *a priori*.

The method is then to tabulate the accessed region of the ILDM. Because the shape and location of this region is not known *a priori*, the table is unstructured and generated *in situ*. Figure 2 provides an overview of the algorithm. It consists of three elements. First, there is a module to perform direct numerical integration of the detailed kinetics as described above. Given a composition ϕ , the module returns the corresponding increment $\Delta\phi$.

Second, there is a data structure in which is stored N pairs of values of composition and the corresponding increment $\{\phi^{(n)}, \Delta\phi^{(n)}, n = 1, 2, \dots, N\}$ of points on the ILDM. The third element is the logic of the algorithm (the middle block in Figure 2).

The logic of the algorithm is simple. If the data structure contains a sample $\phi^{(m)}$ sufficiently close to the given composition ϕ , then we accept the approximation $\Delta\phi \approx \Delta\phi^{(m)}$. Otherwise, $\Delta\phi$ is determined by direct numerical integration, and the pair $(\phi, \Delta\phi)$ is added to the data structure.

3 Report

The sections of this report summarize the accomplishments of the project. More technical details are contained in the two publications stemming from the work (Yang & Pope 1996a, b).

Splitting Mixing and Reaction

Following a fluid particle in gas-phase turbulent combustion, there are two processes that affect the thermochemical composition: reaction, and molecular mixing. While these physical processes occur simultaneously, it is essential to efficient numerical implementations of reaction chemistry that they be treated separately. In other words, a numerical *splitting* is needed.

Some of our tests of the manifold method led to concern that the splitting errors were large. As a consequence we undertook a study of the issue. We ran our PaSR test problem using full kinetics and full coupling of mixing and reaction, and used these results as a standard by which to measure splitting errors. A variety of splitting schemes were investigated from the crudest—mix then react—to different predictor-corrector schemes.

The results shown in Fig. 3 indicate that all of the methods converge linearly with the time step Δt , and in fact, the crudest method (denoted by DS0) is best. (This, possibly surprising, result is due to the fact that the chemistry contains time scales smaller than Δt .)

Manifold Method Solution

The manifold method for incrementing the compositions due to reaction has been further developed and tested. For the same PaSR test as discussed above, also shown in Fig. 1 are the numerical errors in the manifold method. For example, the curve denoted MS0 is the manifold method with the crudest splitting. It may be seen that the method converges linearly as Δt tends to zero, with the magnitude of the error being only twice that with full kinetics. These results confirm that the overall scheme—manifold method with splitting—is accurate: the numerical error converges to zero as the time step is decreased.

The methodology and results on splitting and on the manifold method are fully described in Yang & Pope (1996a).

In Situ Adaptive Tabulation

The most significant accomplishment has been the development of the *in situ* adaptive tabulation (ISAT) algorithm. In this method, the needed reaction information is tabulated *in situ*, as the reactive flow calculation is in progress. Principal directions in the composition space are identified, and the table depends on the first several of these directions.

The method has been tested for a partially-stirred reactor (PaSR) for methane/air combustion with a skeletal mechanism consisting of 16 species and 40 reactions, and for natural gas combustion with the GRI 2.11 mechanism consisting of 49 species and 279 reactions. Results show that this method has excellent accuracy (for all species) and efficiency. A speedup in performing chemistry of four-hundred is obtained for the methane/air combustion system with the skeletal mechanism. The speedup will increase as the calculation continues since less integrations will be performed.

The ISAT method and the tests performed are fully reported in Yang & Pope (1996b).

Interaction with BYU

A student from BYU, Steve Cannon, who is supported by AGTSR spent the Spring 1996 semester at Cornell. The objective of his visit was for him to learn more about PDF methods and manifold methods, so that the BYU AGTSR project will benefit. At Cornell, Cannon is investigating the ISAT algorithm in connection with the simplified chemistry used in the BYU PDF application. The ISAT method has now been implemented in the BYU ACERC code.

Interactions with Industry

The PI continues to interact with Dr. M.S. Anand at Allison Engine Company and Dr. S.M. Correa at General Electric. The communications have concerned the PDF methods in gas-turbine combustor codes and the use of manifold and ISAT chemistry.

4 Publications

Yang, B. and Pope, S.B. (1996a) "An investigation of the accuracy of manifold methods and splitting schemes in the computational implementation of combustion chemistry" Combust. Flame (submitted).

Yang, B. and Pope, S.B. (1996b) "Treating chemistry in combustion with detailed mechanisms—*in situ* adaptive tabulation in principal directions," Combust. Flame (submitted).