GRI-90 / 0116

A Basic Research Model of Gas Combustion in Turbulent Flow

ANNUAL REPORT

(1 June 1988 – 30 June 1989)

Gas Research Institute
8600 West Bryn Mawr Avenue
Chicago, Illinois 60631

GRI-90 / 0116

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A Basic Research Model of Gas Combustion in Turbulent Flow

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GRI Contract No. 5088 - 260 - 1692

Annual Report

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To the
Gas Research Institute

Combustion
Basic Research

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PB91-181
REPORT DOCUMENTATION PAGE | 1. REPORT NO. GRI-90/0116 | 2. | 3. Recipient's Accession No.

4. Title and Subtitle
A BASIC RESEARCH MODEL OF GAS COMBUSTION IN TURBULENT FLOW
Annual Report

5. Report Date

6.

7. Author(s)
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8. Performing Organization Rept. No.

9. Performing Organization Name and Address
The University of Michigan
Ann Arbor MI 48109-2140

10. Project/Task/Work Unit No.

11. Contract(C) or Grant(G) No.
(C)
(G) 5088-260-1692

12. Sponsoring Organization Name and Address
Gas Research Institute
8600 West Bryn Mawr Avenue
Chicago IL 60631

13. Type of Report & Period Covered
Annual Report
June 88-June 89

14.

15. Supplementary Notes

16. Abstract (Limit: 200 words)

This abstract describes the development currently underway of a basic research model for gas combustion in turbulent flow. The model being developed is fundamentally different from the conventional types of turbulence models currently in use for flame calculations, both in terms of the underlying physical approximations made and in the numerical techniques used to implement them. The present approach is based on the idea that many of the precise and detailed fine scale processes at work in turbulent combustion have a simple self-similar structure, and as a result do not need to be continually recomputed in full detail. These can instead be modeled using results from recent experimental research into the fine scales of turbulent flows.

Results obtained to date from this model have been carefully compared with finite difference simulations of the full governing equations for several simple test cases, and show that even complex and highly nonlinear phenomena such as local extinction of reactions in the flow field are correctly reproduced by the model. The model directly incorporates the strong coupling between the fluid dynamics and combustion chemistry in the flame. Work presently underway is incorporating volume source effects into the model. NOx reaction chemistry is also currently being included to allow detailed calculations of NOx formation in various flows. The resulting model will be a new computational tool capable of identifying favorable strategies for NOx reduction and other desired flame properties in turbulent gas flames.

17. Document Analysis a. Descriptors

b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

18. Availability Statement

19. Security Class (This Report) Unclassified | 21. No. of Pages

20. Security Class (This Page) Unclassified | 22. Price

Research Summary

Title	A Basic Research Model of Gas Combustion in Turbulent Flow
Contractor	The University of Michigan (Ann Arbor)
Co-Principal Investigators	Werner J.A. Dahm, Grétar Tryggvason, Robert Krasny
Reporting Period	June 1, 1988 - June 30, 1989
Objective	To develop a physically accurate yet computationally tractable model of gas combustion in turbulent flames by directly incorporating new basic research results for mixing and combustion in turbulent flows into the equations governing fluid motion and chemical reaction. The resulting model will be a computational tool to aid in the development of low NOx flames for the next generation of gas burning applications.
Perspective	Development of the next generation of gas burning equipment for industry and utilities will need to rely more than ever before on detailed computational modeling of the complex physical processes at work in turbulent flames in order to meet the stringent requirements for low NOx emission levels being placed on them. Conventional models of turbulent flames, in which the time-averaged forms of the equations governing fluid dynamics and reaction chemistry are solved using any of a wide variety of gradient transport models, have proven to be unreliable for predicting many sensitive combustion phenomena. Direct computational simulations of the complete time-varying equations, on the other hand, are far beyond the reach of even the largest computers. However, approximate simulations of gas combustion in turbulent flames can be brought within reach by avoiding a fully detailed representation of some aspects of the turbulent combustion process, and instead directly incorporating new results from recent basic research investigations into a computationally tractable yet physically correct model of gas combustion.
Approach	The model under development here is fundamentally different from the conventional turbulence models currently in use for treating gas combustion in turbulent flames, both in terms of the underlying physical approximations and the numerical techniques used to implement them. Our approach is based on the idea that many of the precise and detailed fine-scale processes at work in turbulent combustion do not need to be computed in full detail, and can instead be modeled directly using results from recent basic research investigations. The resulting model is based on Lagrangian tracking of dynamical elements in a turbulent reacting flow to approximately solve the time-varying equations of fluid motion and chemical reaction. Our approach is unique in that the precise internal structure of the vorticity, density, temperature, reactant and product concentration profiles

within the flow do not need to be computed, and are instead specified directly as families of self-similar shapes characterized by a finite number of degrees of freedom. Moments of these profiles are then allowed to evolve to satisfy the equations of fluid dynamics and reaction chemistry. The resulting model can accurately simulate combustion in turbulent flows and is far simpler and faster than other methods, allowing detailed computational modeling of even very complex processes in turbulent gas flames.

Results

A new and very general integral method has been developed that directly treats the molecular diffusion and chemical reaction processes occurring at the finest scales of the flow. This submodel greatly reduces the number of elements that need to be tracked in such a Lagrangian calculation, thereby allowing a corresponding increase in the complexity of problems that can be computed. The model makes direct use of recent experimental results showing that molecular diffusion occurs in locally self-similar strained laminar diffusion layers throughout a turbulent flow and allows such physically important processes as differential diffusion to be directly incorporated.

Results from this integral submodel for molecular diffusion and chemical reaction have been carefully checked in numerous test cases for a time-varying strained diffusion and reaction layer, and show good agreement with full finite difference calculations. In these test cases, the integral method shows a factor of more than 100 reduction in the computational effort required for such problems. The submodel has been shown to correctly reproduce even highly sensitive nonlinear features of the reactions, including extinction and re-ignition of large Zel'dovich reaction kinetics.

A fluid dynamics code based on Lagrangian tracking of vortex elements has been implemented. Consistent with the diffusion and reaction model described above, this method uses single vorticity elements to represent the entire normal structure of vorticity layers in the flow. This differs from many other Lagrangian tracking methods that use several elements in an attempt to accurately determine the precise inner structure of such vorticity layers at the expense of large increases in computational time.

Results from this fluid dynamics model have been checked against full Navier-Stokes calculations in benchmark tests to assess the accuracy of this representation. Key features of the flow field evolution, including such sensitive measures as strain rate maps, are found to be reproduced by the model in a small fraction of the computational time. Three-dimensional calculations using this fluid dynamics model have also begun.

The fluid dynamics code has been successfully combined with the molecular diffusion and chemical reaction submodel to calculate the evolution of gas combustion in turbulent flows. Results from this combined model are currently being compared with finite difference solutions of the full governing equations for several simple test cases, and show that even complex phenomena such as local strain-out of reactions in the flow field are tracked with errors of typically less than a few percent. The combined

code can in principle treat cases that are well out of reach of such full finite difference simulations.

NOx calculations using this model have begun in order to show where the nitric oxide forms in the flow field and from this to suggest new strategies for NOx reduction in turbulent flames. At present, a simple one-step kinetic formulation is being implemented. More realistic kinetic representations for the NO reaction chemistry are planned.

Project Implications

This research is aimed at developing a computational tool applicable to turbulent natural gas combustion. The model recognizes that many of the detailed fine scale turbulent combustion processes are now relatively well understood and do not need to be continually recomputed. The model calculates the flow field directly, rather than attempting to use scaling laws specific to a particular flame type. Thus, the model is capable of assessing flame properties, including the NOx emissions, for a broad class of combustion applications. This model, based on contractor's understanding of and insight into the physics of turbulent combustion, has very good potential as a tool to simulate turbulent combustion faster than conventional methods. When completed, the model will be able to accurately simulate the complex processes in turbulent natural gas flames. This study is an important part of GRI's work to develop a model for practical turbulent natural gas flames.

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1.0 Overall Program Objectives

This basic research program is a combined theoretical and numerical effort with the following three major objectives:

1. To *incorporate* new basic research knowledge resulting from GRI's combustion research program in turbulent flames into physically correct submodels of the underlying fluid dynamics and combustion processes in turbulent gas flames,

2. To *develop* these individual submodels into a complete computational code capable of accurately modeling the complex and highly detailed gas combustion process in turbulent flames,

3. To *use* the resulting computational code as a new basic research tool to help develop innovative strategies for achieving NOx reduction in turbulent flames.

The long range purpose of this research effort is to produce an entirely new type of turbulent flame model that can be reliably used as a design tool to help meet the stringent combustion requirements being placed on the next generation of gas burning equipment for industry and utilities.

2.0 Overview of Present Modeling Approach

2.1 Background

In order to promote development of new gas burning markets through design of low NOx turbulent flames for gas burning applications in industry and utilities, a computational tool will be needed to allow accurate and reliable assessment of the effects of potential design innovations on the resulting flame properties. It might seem that the development of such a computational tool would be a straightforward matter, since the complete governing equations that determine fluid motion and reaction chemistry in turbulent gas flames are well known. However at present, and for the foreseeable future, the computational requirements needed for numerically solving these governing equations for turbulent flames far exceed the capabilities of even the most powerful of modern computers. For this reason, the numerical calculation of combustion in turbulent flames has instead traditionally been based on the *time-averaged* versions of these governing equations, the mathematical nature of which requires that *turbulence modeling* must be incorporated into such calculations in order to allow these equations to be solved.

Numerous such turbulence models have been developed over the past 50 years, but all of these are in fact minor variations on the same underlying physical idea first proposed by J. Boussinesq in 1877, namely the *assumption* that mixing between the fuel and oxidizer in turbulent flames is a *gradient transport* process. However, such traditional turbulent flame codes, all of which ultimately are based on this assumption, have proven to be unreliable for predicting in advance many of the most important and sensitive combustion phenomena resulting from major innovations in the design of gas burning equipment, including such crucial flame properties as in-flame NOx levels and flame stability limits. As a consequence, while such conventional flame codes are presently the only resort for designers of industrial burners and furnaces, their rather limited reliability restricts their use to relatively small modifications around the traditional design concepts for which these codes have been 'tuned'. As a consequence, and most importantly, these conventional codes do not allow exploration of genuinely innovative and comparatively radical design changes that might be profitable for achieving desired turbulent flame properties, such as NOx reduction, increased flame stability, and increased flame radiation.

Extensive research into combustion in turbulent flames over the past ten years, supported in part by GRI's Basic Research Program in Combustion, has shown why this conventional approach to modeling turbulent flames is unreliable for predicting many effects of major departures from traditional designs of gas burning equipment. In particular, this body of work has shown that the gradient transport assumption which forms the basis of such conventional turbulent flame codes is physically *incorrect* and is the major reason for their unreliability. This research work has also given new insight into the correct and detailed physical processes governing mixing and combustion in turbulent flames from precise laboratory study of turbulent flows and combustion within them under very carefully controlled conditions. Moreover, much of this research work has also been aimed at understanding how these physical processes scale up from small scale laboratory flames to the large scale flames typical of industrial combustion applications. As a result, this basic research program has accumulated a detailed base of new knowledge about the *correct* physical processes that govern combustion in large scale industrial turbulent flames, which can now be assimilated to form an entirely different class of computational models for such flames.

Indeed, the strict requirements for low NOx emission levels that are currently being placed on gas burning applications in many parts of the country suggest that significant departures from traditional design practices will likely be needed to meet these stringent demands, and will require a capability for analyzing the complex and detailed physical processes governing combustion and NOx formation in turbulent flames.

- *This suggests that development of the next generation of gas burning equipment for industry and utilities will need to rely more than ever before on detailed computational modeling of the complex physical processes at work in turbulent flames, and that this will require an entirely new class of turbulent flame models as a design tool for giving reliable assessments of NOx levels and other flame properties.*

The objective of this work is to produce such a model that can be reliably used for detailed calculations of gas combustion in turbulent flames to identify new strategies for achieving NOx reduction and other flame properties in gas burning applications.

2.2 Overall Modeling Approach

The goal of the modeling work described in this report is to provide such a computational tool to meet the requirements being placed on current and future gas burning applications. It is essential to note from the outset that the turbulent flame model under development here is fundamentally different, both in terms of the underlying physical assumptions on which it is based and the numerical techniques used for their implementation, from the conventional turbulence models commonly used for treating combustion in turbulent flames.

In particular, our model is not based on the time-averaged versions of the complete governing equations for fluid motion and combustion chemistry. Instead, as outlined in Figure 2.1, the model directly incorporates physically correct approximations motivated by this new understanding of the fundamental physics of gas combustion in turbulent flames, obtained in part from GRI's basic research program, together with other physically justifiable approximations, into the complete governing equations to bring them within reach of current computational capabilities.

- *The underlying theme behind our model development is that many of the detailed fine-scale processes at work in turbulent combustion are comparatively well understood and do not need to be continually recomputed in precise detail. Indeed, experiments show that these processes have a self-similar structure to them that can be approximately incorporated directly into the complete governing equations to bring the modeling of turbulent flames within computational reach.*

This can greatly simplify the complexity associated with computational modeling of turbulent flames, and we have developed these types of approximations into a new type of model for gas combustion in turbulent flames. At the same time, we have conducted careful and detailed comparisons with numerical solutions of the complete equations for several simple configurations to allow a thorough understanding of the physical nature of the approximations made and the level of accuracy achieved, as well as a documentation of the reliability represented by this model.

- *Rather than hastily producing crude model results that merely 'look turbulent' but are physically incorrect or which lead to a model that is computationally prohibitive, the approach to modeling adopted here is instead based on developing a foundation of new, physically motivated, carefully tested, and well understood simplifying approximations that will produce a model which can be reliably used to assess gas combustion in turbulent flames.*

- *We also believe that the resulting model must be a very general tool capable of assessing the NOx output and other flame properties of a wide class of combustion applications, and should not be applicable only to one specific type of flame or to a narrow class of flames.*

As is shown schematically in Figure 2.2, our complete model for numerically determining the entrainment, mixing and combustion processes in turbulent flames is separated into *(i)* a Fluid Dynamics Model for determining the flow field, and *(ii)* a Combustion Model for treating the molecular mixing and chemical reactions occurring in the flow. A brief overview of the Combustion Model is given in §2.3 below, and a detailed technical description of this model together with a presentation of typical results achieved to date is given in §3 of this report. Similarly, an overview of the Fluid Dynamics Model is given in §2.4 below, and a detailed technical description including typical computational results is given in §4 of this report. The coupling between these Fluid Dynamics and Combustion submodels, which is also shown schematically in Figure 2.2, is summarized in §2.5 below and is described in greater technical detail in §5 of this report.

Each of these submodels is based on grid-free Lagrangian tracking of various dynamical elements which satisfy the time-varying governing equations of fluid motion and chemical reaction, as is detailed in this report. The results from this basic research model of the fluid dynamics and combustion processes in turbulent flames, including such detailed information as the reactant, product and temperature fields as well as the associated NOx distribution, soot loading in the flame and heat radiation from the flame, then serve as inputs to industrial burner or furnace models, as also shown in Figure 2.2.

2.3 Combustion Model

The combustion submodel tracks the evolution of the molecular mixing and chemical reaction among all relevant chemical species fields, as well as the associated temperature field, throughout the region of interest in the flow. This is accomplished with a new local integral method, developed during the past year under this contract and outlined in detail in §3 of this report (see also Tryggvason & Dahm 1989), which allows the chemical species conservation equations to be solved up to *several orders of magnitude faster* than if conventional methods, such as finite differences, were used.

The physical basis of this new method is the recent experimental observation from highly detailed imaging measurements (Dahm & Buch 1989, 1990) that the internal species profiles within the strained laminar diffusion layers in turbulent flows are essentially self-similar. As a consequence, it is not necessary to continually recompute the internal structure of the species profiles within these layers, and instead these can be specified as a family of self-similar profile shapes with any desired number of degrees of freedom. The corresponding integral moments of the local temperature profile as well as all local chemical species profiles are then evolved in time to satisfy the parabolized forms of the complete governing species conservation equations and the energy equation subject to the local strain rate history determined from the fluid dynamics submodel. This removes the need to solve a partial differential equation and replaces it with an ordinary differential equation, with a corresponding increase in computational efficiency. Each of the individual species concentration fields can then be reconstructed from these integral moments using a fast boundary integral method.

This combustion model has been applied to a wide range of test cases and compared with results from fully detailed finite difference solutions of the complete governing equations. Many of these comparisons are presented in detail in §3. The results show that it is capable of modeling the evolution of species in such diffusion and reaction layers under strongly time-varying strain rate fields, as would be encountered in turbulent flames, with results typically within a few percent of full finite difference calculations. These test cases also verify that the model accurately accounts for the interactions among adjacent diffusion and reaction layers. Moreover, this combustion submodel has also