Summer Work Experience: Determining Methane Combustion Mechanisms and Sub-scale Diffuser Properties for Space Transportation System Engine Testing

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Abstract

To assess engine performance during the testing of Space Shuttle Main Engines (SSMEs), the design of an optimal altitude diffuser is studied for future Space Transportation Systems (STS). For other Space Transportation Systems, rocket propellant using kerosene is also studied. Methane and dodecane have similar reaction schemes as kerosene, and are used to simulate kerosene combustion processes at various temperatures. The equations for the methane combustion mechanism at high temperature are given, and engine combustion is simulated on the General Aerodynamic Simulation Program (GASP).

The successful design of an altitude diffuser depends on the study of a sub-scaled diffuser model tested through two-dimensional (2-D) flow- techniques. Subroutines given calculate the static temperature and pressure at each Mach number within the diffuser flow. Implementing these subroutines into program code for the properties of 2-D compressible fluid flow determines all fluid characteristics, and will be used in the development of an optimal diffuser design.

Introduction

Cryogenic rocket testing at the NASA-Stennis Space Center (SSC) three-celled Component Test Facility includes rocket engine component evaluations using liquid oxygen, hydrogen and hydrocarbon fuels, solid or hybrid rocket motor testing, and other testing involving high flow rate and high-pressure fluids. SSC researchers use the Component Test Facility to advance knowledge in engine test technology, instrumentation, and component design.

As a NASA Undergraduate Student Research Program (USRP) Scholar and NASA-GEM Fellow, I worked in the Propulsion Test Division under the guidance of

NASA-SSC Chief RLV Engineer Gerald Pitalo for two summer internships. During these two internships, I worked on two major projects related to the research and development of the Space Transportation System Engine component design. Specifically, the projects involved researching 1) the use of methane and dodecane to fuel the STS Engine, and 2) the modeling of a sub-scaled self-pumping altitude diffuser using 2-D flow techniques.

Project I

Objective

The Space Shuttle Main Engine uses liquid hydrogen and oxygen to propel the Space Shuttle into space. Other rocket engines use propellants such as kerosene, hydrogen, oxygen and other hydrocarbons. My mentor, Mr. Pitalo, studies the characteristics of kerosene as a possible propellant for future STS Engines. Since methane and dodecane have similar reaction schemes as kerosene, they are used to simulate kerosene combustion processes at various temperatures. As an intern, I assisted in researching methane and dodecane oxidation models. With the chemical oxidation reactions of methane and dodecane documented, engine combustion is simulated on the General Aerodynamic Simulation Program (GASP). Initial conditions, object code and zonal boundaries must be inputted into GASP to simulate the combustion process.

Investigation

This project was based on the chemical equations of methane (CH_4) combustion. Review in organic chemistry and chemical kinetics was necessary to understand hydrocarbon combustion. After reading several texts regarding methane combustion and high temperature combustion of alkanes, it was found that when methane combusts, it initiates a chain of chemical reactions. These combustion processes, or mechanisms, include several equations that describes methane's chemistry. (Figure 1)

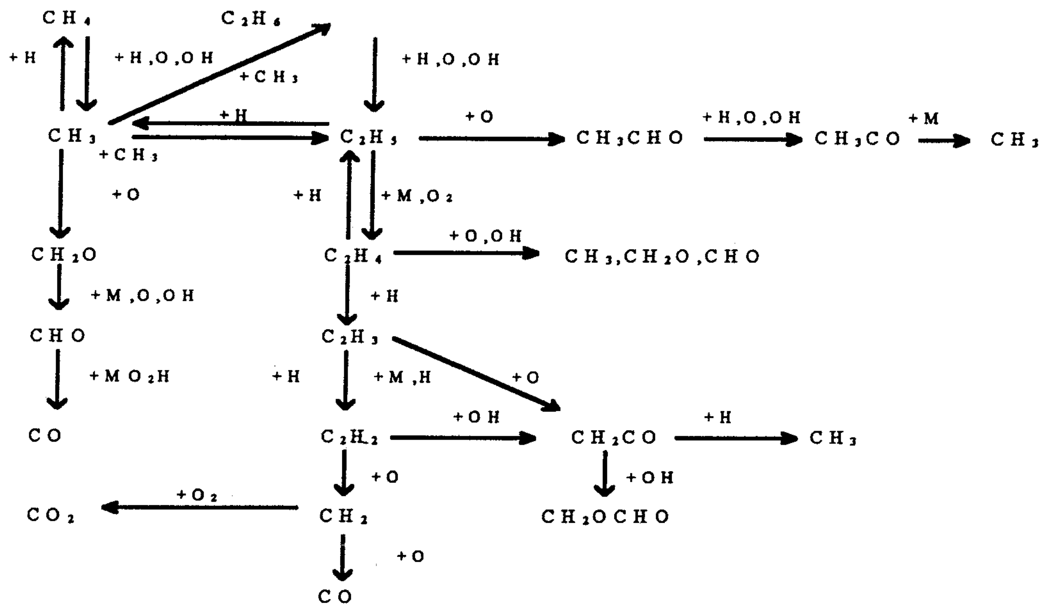

Figure 1: Warnatz Mechanism methane combustion[1]

During the oxidation of methane, low temperatures induce low energy, which decreases the number of reactions. However, at high temperatures the rates of initiation process increases, thereby producing a higher number of hydrogen and oxygen species. Although the methane combustion process is the simplest hydrocarbon fuel, it has a complicated branched chain reaction.

The subroutines for the methane combustion mechanism at high temperatures were calculated using the National Institute of Standards and Technology (NIST) Chemical Kinetics database. By identifying the main chemical equations, this information is used to detect details of kerosene combustion. Using the mechanism for methane, I recorded the activation energy (Ea), temperature range (T), and frequency factor (A) and other variables found in NIST. Later, I calculated the reaction rates for over 342 chemical reactions were calculated using the Arrhenius equations:

$$k(T) = A \exp(-Ea/R * T) \qquad (1)$$

$$k = A(T/298)n * \exp(-(Ea/R)/T) \qquad (2)$$

where R = 8.31441 e-3 kJ/kg-mole. These reaction rates will be used in the GASP code to simulate methane combustion in the engine combustion chamber.

The results of this project included the extraction of reaction rates from the NIST database based on the Warnatz methane combustion model. (Figure 2) Two technical summaries relating to methane kinetics in supercritical water [2,3] were reviewed and written. Initial dodecane research began with the contact of Exxon representatives and Stanford University Mechanical Engineering Professor Reginald Mitchell. Finally, research reports were ordered from the Maury Naval Library for future analysis of the dodecane mechanism.

Reactants 1 & 2	Chemical Equation	Reaction Rate Linear	Reaction Rate Non-Linear	Temperature (K)
CH_4 + H	H + CH_4 -> H_2 + CH_3	1.08e+13	3.48e+13	2500
CH_4 O	CH_4 + O -> Products	1.47e+10	1.479e+10	583
	O + CH_4 -> OH + CH_3	1.58e+13	3.087e+13	2575
CH_4 OH	OH + CH_4 -> H_2O + CH_3	1.13e+13	4.37e+13	3000
CH_3 + CH_3	CH_3 + CH_3 -> Products	4.41e+12	N/A	2000

Figure 2: Partial listing of Methane Mechanism of Combustion using Warnatz 1981 and 1984 model and NIST at high temperatures

Conclusion

Methane's complex combustion mechanism at high temperatures provide a template on how to model the kerosene combustion process. Little research relating to kerosene and dodecane combustion exists because of their complicated reaction process. However, by analyzing the methane mechanism and implementing the subroutines into GASP, Space Transportation System Engine combustion is simulated. Further investigation on the dodecane combustion model must be completed to evaluate its properties and mechanisms in GASP.

Project II

Objective

The rocket engine facilities at the NASA-SSC use self-pumping altitude diffusers to simulate altitude at the exit plane of the Space Shuttle Main Engine. An altitude diffuser is attached and sealed around the SSME to simulate the low-pressure environment experienced during Space Shuttle ascent. Currently, the A-2 stand diffuser at SSC has been used for 25 years, and it was discovered that thermal stresses produced cracks in the diffuser's lower section. It is anticipated that the determination of flow conditions and shock structures will predict diffuser hardware deterioration. Once a sub-scale diffuser model is created and tested through 2-D flow techniques, cost effective and reliable materials will be selected.

At SSC, an on-going research effort has been established to identify critical operational and cost effective designs. Engineers search for diffuser designs that are reliable, operable, and easy to maintain. Mr. Pitalo and Professor Christopher Cho from Western Michigan University recently simulated a sub-scaled self-pumping altitude diffuser using supersonic one-dimensional 1-D flow techniques[4]. Using this information, the primary goal of my project was to apply the method of characteristics to 2-D altitude diffusers for SSME testing. Method of characteristics include the partial differential equations necessary to determine the design diffuser characteristics at high temperatures. Specifically, I was to find the appropriate environment flow, shock, and 2-D gas dynamic conditions used. This information will be used to analyze a small sub-scale model of a self-pumping altitude diffuser and to predict its temperature profile using the 2-D techniques.

Investigation

To help find an optimal self-pumping diffuser, research was conducted on information relating to diffuser design using supersonic 2-D flow techniques. Before the application of the 2-D flow techniques could be used, properties of 1-D flow for the model were reviewed for the design of the sub-scaled diffuser. According to the design, the sub-scaled diffuser inlet will be approximately 6 inches in diameter, and will be attached to the engine nozzle exit.

This design of this project was based on the method of characteristics, which are equations that apply to both 1-D unsteady flow and 2-D steady flow. Preparation for this project included the review of engineering and mathematical solutions and general fluid mechanics problems. To begin my work on 1-D compressible flow, the study of the definitions of isentropic flow, normal shock, and choking was done. Careful review of equations and examples relating to the calculations of these properties was completed. To become familiar with the 1-D diffuser design process, I analyzed 1-D data for design of the DTFT (Diagnostic Testbed Facility Thruster) Diffuser calculated by Dr. Cho[5].

Thereafter, I examined engineering problems and calculations relating to 2-D compressible flow. SSME diffuser cases and papers relating to the endurance of a diffuser under severe rocket engine conditions were available for my study. To write the code that calculates the temperature and pressures within a nozzle, reference was given to an engineering problem similar to the calculation of nozzle flow characteristics. The coding for this problem assisted me in understanding the process of designing a subroutine, which can calculate the Mach number, static pressure, temperature, and Prandtl-Meyer angle at a given coordinate, or lattice point, within an engine.

Results

The final output of my summer research included the calculations of static temperature and pressure at each Mach number within the engine flow. (Figure 3) This flow is also known as a Prandtl-Meyer flow, where supersonic flow turning through a convex corner expands the flow. The resulting properties increase in velocity and decrease in pressure. Assumptions of this flow include isentropic stagnation properties of an ideal gas.

Additional project results include coding subroutines in FORTRAN 77 programming which calculate static pressures and temperatures. These subroutines will be implemented in Dr. Cho's program code for determining all the properties of 2-D compressible fluid flow in the altitude test diffuser. Once the program is completed, all characteristics of the fluid flow in the diffuser are determined and an optimal design developed.

Mach Number	Pressure (psi)	Temperature (°R)
1.43	30.12	709.7
1.59	23.88	664.18
1.74	19.07	622.85
1.90	14.92	580.7
2.06	11.64	540.9
2.23	8.92	501.36
2.41	6.73	462.62

Figure 3: Sample calculations of pressure and temperature at each Mach number for total conditions.

Conclusion

The design of a sub-scale altitude diffuser uses method of characteristics for supersonic flow. The method of characteristics is a method applied to 2-D flow to determine how temperature, pressure, and other properties change with mach number. The properties of the flow are determined at various points, or lattice points, within the engine nozzle. After discussion with Dr. Cho, it is concluded that when the lattice points increase, more accurate information about the static temperature and pressure for 2-D supersonic flow are found for each Mach number. Increasing lattice points in the method of characteristics to analyze other cases, such as water injected at the diffuser inlet, is recommended.

Acknowledgment

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