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COMPUTATIONAL MODELING OF MULTI-PHASE/MULTI-SPECIES FLOWS WITH APPLICATIONS TO LIQUID ROCKET ENGINES

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Accurate prediction of all physical phenomena in a combustion chamber is essential for better understanding of the system performance. Atomization, evaporation, combustion, chemical kinetics, and turbulence are those processes of great importance that need to be well understood. Processes involving the liquid phase in a combustion chamber will be further complicated under supercritical conditions. More advanced and accurate numerical techniques are required to extend our understanding of the above phenomena. A computer program for multi-species/multi-phase flow was developed for NASA/MSFC in 1992. This code, called Liquid Thrust Chamber Performance (LTCP) program takes an Eulerian-Eulerian approach and is based on the Total Variation Diminishing (TVD) technique with Lax-Friedrichs upwind method. Under the NASA/ASEE SFFP the LTCP code was used to predict the performance characteristics of several engines that were of particular interest to NASA. This code was also successful in a combustion detonation study. Converting the program to the PC platform was accomplished which extends usability and makes it available to a wider range of users. The Eulerian formulation of the liquid phase provides a suitable model that can be extended to include combustion modeling under supercritical conditions. The results have been compared against the ones of other codes and available measured data. The algorithm proved to be robust and efficient for problems with stiff source terms.

1.0 INTRODUCTION

Since the inception of Computational Fluid Dynamics (CFD), enormous effort has been directed toward developing an efficient and robust algorithm for stiff systems. In spite of impressive progress in these developments for pure substances, solving the coupled equations for multi-phase systems with stiff interphase interaction and chemical reactions still remains a challenge.

Most CFD solutions for such systems are obtained by ad hoc methods that deviate from the actual problem in hand, either by introducing unfounded assumptions or over-simplifying the governing equations. Some CFD codes separate the species continuity equations from the rest of the conservation equations, which yield an overdamped or

unstable system. To overcome the stability problem, an excessive damping is frequently introduced in the equations which can potentially generate a non-physical solution. Some CFD codes that are designed for two phase flows "minimize" the number of source terms that represent the inter-phase interaction. These terms will cause momentum and energy "spikes" which can trigger instability. Most of the Navier-Stokes (NS) solvers do not have a comprehensive chemical reaction mechanism to allow for the evaporation of fuel and/or oxidizer droplets, which permits them to proceed with the chemical kinetics to generate combustion products. In other words, they assume that the droplets in the gaseous phase immediately react and reach an equilibrium state.

The LTCP code was developed under a NASA/MSFC contract based on the philosophy of "minimizing" the formulation "compromises". As a consequence all the inter-phase interaction terms are included. The evaporation models and fully-coupled finite rate chemistry permit the proper combustion modeling. The Eulerian approach was selected for the liquid phase to make the code suitable for dense spray combustion simulation.

2.0 MATHEMATICAL FORMULATION

The governing equations for the gas and liquid phases are given in Reference (1). Due to their extent and complexity, they will not be repeated here. The species production/destruction terms resulting from chemical reaction and evaporation are all included in the source term. It should be mentioned that in an Eulerian framework a "continuity" equation for the droplet radius change must also be contemplated. Some researchers[2] have chosen to solve the equation for the droplet radius change in a Lagrangian framework to avoid singularities which will be caused by very small droplets.

3.0 NUMERICAL MODEL

The conservation equations are linearized with respect to the following vector:

$$\mathbf{Q} = [u, v, T, P_1, P_2, \ldots, P_N, k, \varepsilon]^T \qquad (1)$$

where $P_N=C_NP$, with P being the static pressure, and C's are species mass fraction. P_N is referred to as "pseudo partial pressure". The significance of using the above vector is in achieving robustness for flows at "all speeds". That means the solver must be equally efficient for low speed as well as supersonic speed. For the droplet phase this vector has the following form:

$$\mathbf{Q} = [u, v, \rho, R, T]^T \qquad (2)$$

The Total Variation Diminishing (TVD)[3,4] method is used to evaluate the fluxes for the left and right states. The Lax-Friedrichs[3,4] (LF) upwind technique is used in combination with TVD. The Steger-Warming[1,4] flux splitting is employed for the droplet phase

equations. The details of the chemistry and evaporation model can be found in Reference (1).

4.0 TEST CASES AND DISCUSSION

Numerous test cases of interest to NASA were considered. From the many studies conducted in our research effort, some selected results for three testcases are presented, and the remaining ones are tabulated in Table 1. More pertaining information can be obtained from Mr. Klaus W. Gross at NASA/MSFC.

Table 1 Test Case Matrix

Test Case	Conditions*
1. Space Shuttle Main Engine (SSME) - Flowfield Variation Analysis - Finite Rate Chemistry with O_2/H_2 - Striation with O_2/H_2	 Pc=3000 and 6000 psia, Ideal Gas Pc=3000 psia, Tc=6215 °R, O/F = 6.0 Pc=3000 psia, $(O/F)_{wall}$=4 (1%), $(O/F)_{core}$=6
2. RD0120 Engine, O_2/H_2	Pc=3171 psia, Tc=6514 °R, O/F=6
3. 60k Motor, RP-1/O_2, 8 Species Reaction	Pc=651 psia, Tc=6391 °R, O/F = 2.34
4. Solar Engine, H_2	Pc=20 psia, Tc=4900 °R
5. Non-Premixed Gas Flow Single Injector with Wall Cooling H_2/O_2 Combustion 6 Species Reaction	H_2 Stream Conditions: T = 180 °R U = 656 ft/sec At the Wall: T = 540 °R U = 492 ft/sec
6. Premixed Two-Phase Flow Single Injector RP-1/O_2 Combustion 22 Species Reaction	RP-1: T = 300 °R LOX: 180 °R N = 2.5x10^4/cc 5x10^4/cc U = 50 ft/sec 50 ft/sec D = 100 μm 100 μm
7. Pulsed Detonation Problem O_2/H_2	Initially: P=14.7 psia, T=540 °R, O/F=8 Pulse: T=5400 °R

*Pc and Tc are respectively chamber pressure and temperature, O/F or MR (mixture ratio) the oxidizer/fuel mass flow rate ratios. N is the number density per cubic centimeter, D is the initial droplet diameter

Figures 1 through 4 show the results consisting of temperature and species contours for the testcase 5. It can be seen that hydrogen and oxygen start to react after a short distance downstream of the injector. The flame is concentrated at the hydrogen and oxygen interface. This testcase was selected from Reference 5, where flow measurements and visual data information are available.

Figures 5 through 8 demonstrate the Mach number, Temperature, and some selected species contours for the premixed RP1/LOX testcase No. 6. Both liquids enter the combustion chamber in form of droplets. A total of 22 species were considered for the finite rate chemistry. It appears that after a short distance from the injector face an spontaneous combustion occurs which is attributed to the chemical reactions. Therefore, the temperature rises and due to these rapid changes a pressure wave is generated. One of

the disadvantages of hydrocarbon based fuels are the amount of carbon monoxide that is generated by the combustion process. At fairly "high" mixture ratios (>2.0) the possibility of soot production is reduced considerably, therefore, our model did not account for a soot formation mechanism. However, the model is quite capable of such modeling.

Figures 9 shows six time snapshots of the pressure field as a detonation pulse wave propagates in a duct. For this test case a total of six species and eight step chemical reactions were considered. Figure 10 demonstrates the pressure variation as a function of distance along the length of the channel. A peak pressure of about 290 psia was observed. Figure 11 shows the pressure and temperature history on the center of the left wall. Initially, the temperature is suddenly raised to 5400 °R while the pressure is at 14.7 psia. However, after a very short time the pressure starts to rise and at the same time the temperature will increase in an attempt to reach to the adiabatic flame temperature.

5.0 CONCLUSION

The results of this research effort demonstrated that the TVD-LF algorithm is robust and efficient in treating problems with stiff source terms. The Eulerian formulation for the droplet phase was suitable for dense spray combustion and the numerical difficulties were overcome by a fully coupled approach and an implicit Steger-Warming algorithm. Further work is necessary to enhance the capabilities of the LTCP code. The "pseudo time accurate" option of the LTCP code for detonation or ignition studies should be upgraded to a "true time accurate" solution. The higher-order terms for computation of the aeroacoustics must be included in the code for better capturing of the primary pressure wave and some of the harmonics. A fourth-order accurate methos in space and time, is recommended to perform such studies.

6.0 REFERENCES

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2. Chiu, H.H. and X.Q. Zhou, GEMCHIP-CODE: Spray Combustion Process in Airbreathing Propulsion Applications, University of Chicago, Ph.D. Thesis, 1983.
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4. Dang, A.L., Navaz, H.K., and R.H. Rangel, "Numerical Analysis of Bipropellant Combustion in Liquid Thrust Chambers by an Eulerian-Eulerian Approach", AIAA Paper No. 92-3735, 1992.
5. Mayer, W., Schik, A., Schweitzer, C., and M. Schaffler, "Injection and Mixing Processes in High Pressure LOX/GH_2 Rocket Combustor", AIAA Paper No. 96-2620, 1996.

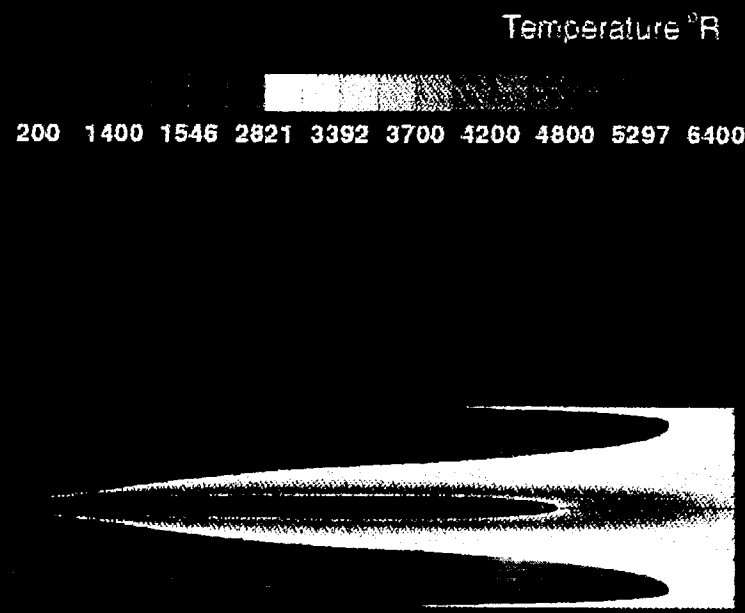

Figure 1 Non-Premixed GO_2/GH_2 Temperature Contour for Single Element Combustion

Figure 2 H_2 Mass Fraction Contours for Non-Premixed GO_2/GH_2 for Single Element Combustion

Figure 3 H_2O Mass Fraction Contours for Non-Premixed GO_2/GH_2 Single Element Combustion

Figure 4 O_2 Mass Fraction Contours for Non-Premixed GO_2/GH_2 Single Element Combustion

Figure 5. Mach Number Contours for Premixed RP1/LOX with 22 Species

Figure 6. Temperature Contours for Premixed RP1/LOX

Figure 7. H_2O Mass Fraction Contours for RP1/LOX

Figure 8. Carbon Monoxide Mass Fraction Contours for RP1/LOX

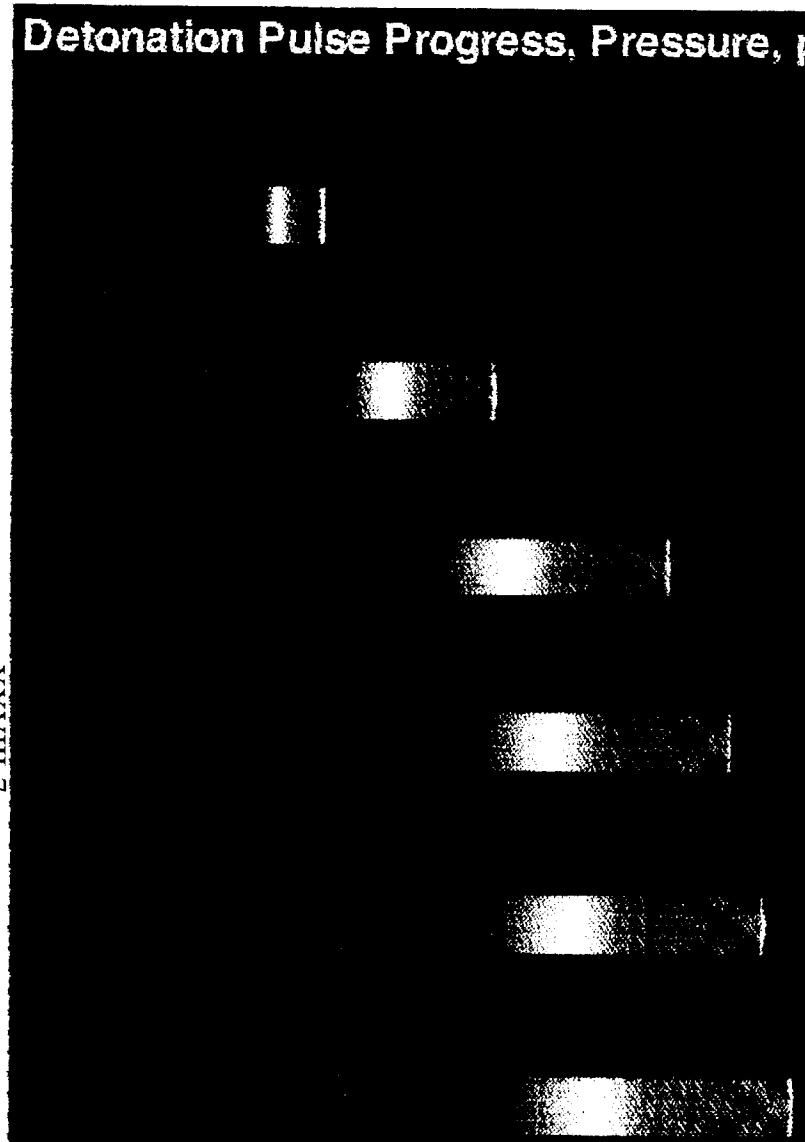

Figure 9. Detonation Pulse Progress in Time
Initial Pressure = 14.7 psia,
Initial Temperature = 540 °R
Temperature Raised to 5400 °R

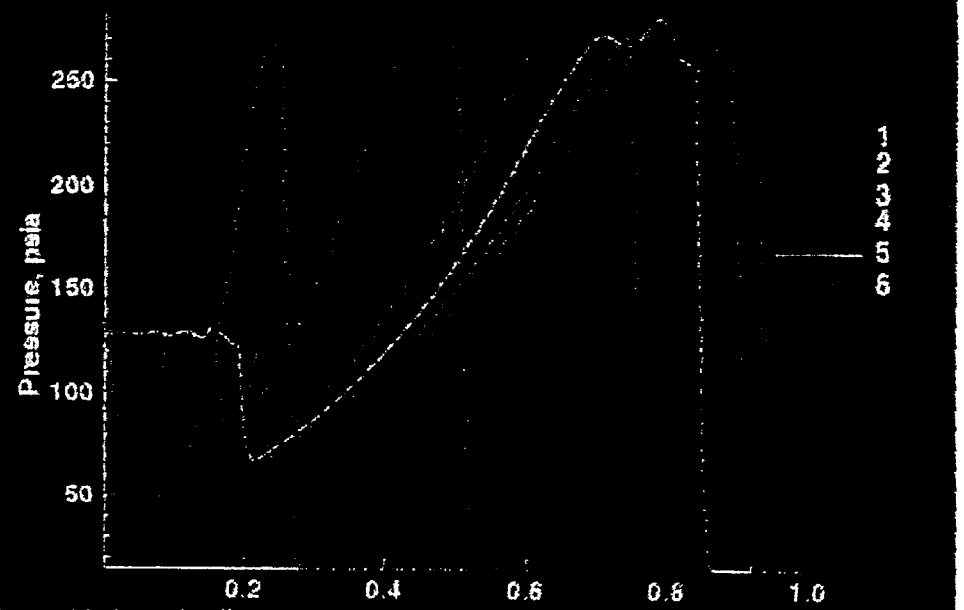

Figure 10. Longitudinal Variation of the Static Pressure for the Six Snapshots

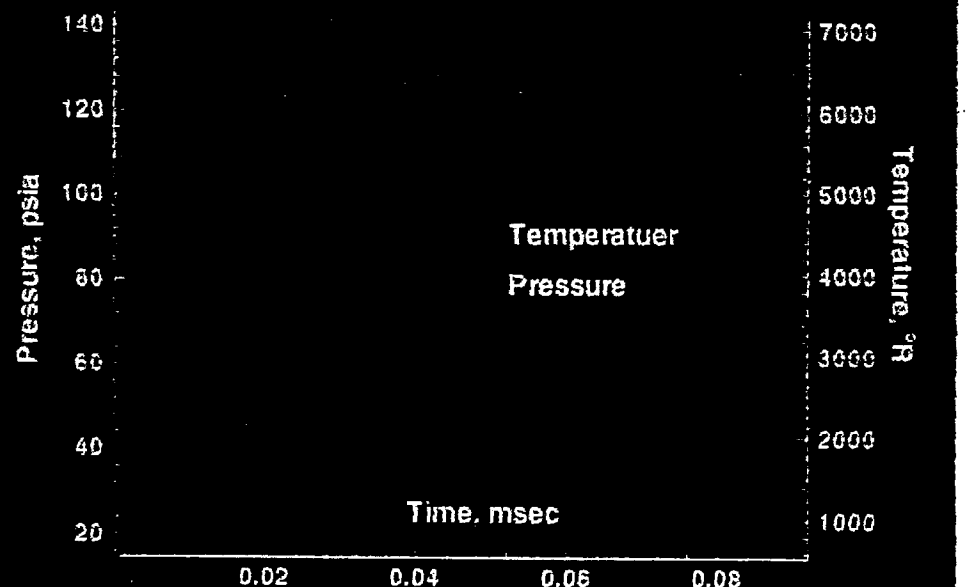

Figure 11. Pressure and Temperature History on the Left Wall