1992

NASA/ASEE SUMMER FACULTY FELLOWSHIP PROGRAM

MARSHALL SPACE FLIGHT CENTER
THE UNIVERSITY OF ALABAMA

COMPUTERIZED REDUCTION OF ELEMENTARY REACTION SETS FOR CFD COMBUSTION MODELING

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1. Introduction

Modeling of chemistry in Computational Fluid Dynamics can be the most time-consuming aspect of many applications. If the entire set of elementary reactions is to be solved, a set of stiff ordinary differential equations must be integrated. Some of the reactions take place at very high rates, requiring short time steps, while others take place more slowly and make little progress in the short time step integration.

Historically, the problem has been approached in several ways:

1) Single Step - Instantaneous Reaction: While computationally simple, this technique will over-predict conversion since the equilibrium point will be surpassed.

2) Total Equilibrium: This is the assumption used in ODE and TDE at MSFC. The assumption may be adequate in describing the overall performance of an engine, but may fail to provide the detail required for the spatial resolution which CFD analysis is to provide. That is, the assumption may not be valid for the local conditions resulting from the CFD calculations.

3) Reduced Mechanism - Finite Rate: The choice of the appropriate reduced set is difficult, since the local conditions are not constant throughout the CFD calculations. Since the importance of the elementary reactions may change within the computational space, the global set chosen may not be appropriate for the local conditions.

4) Partial Equilibrium - Finite Rate: A portion of the reactants are assumed to be in equilibrium, while the remainder are integrated in finite rate kinetics. This approach removes the very short time step calculations and allows integration of fewer equations at longer time steps. Since there is an interaction between the equilibrated and non-equilibrated species, an equilibrium calculation is performed at each time step. KIVA (Los Alamos) utilizes this approach. However, the proper choice of equilibrated and non-equilibrated reactions may change with the local conditions.

The goal of this work is to develop a procedure to automatically obtain sets of finite rate equations, consistent with a partial equilibrium assumption, from an elementary set appropriate to local conditions. The sets can be applied to the appropriate regions within the CFD space where the total equilibrium assumption is inappropriate.

2. Approach

A program was successfully run using the entire combustion chamber as a single cell in the summer of 1991. (Wikstrom, 1991) While the reduced reaction set should be adequate to predict the overall performance of the combustion chamber, the test of applicability requires variation within the combustion space. The conditions for the reduction were to be chosen from a CFD solution in which the local temperature and mixture ratio varied with the combustion solution. In order to find such a solution, a two phase model of the combustion was used, and in order to demonstrate the value of the technique, hydrocarbon fuel, with its more complicated chemistry was selected.

Coinciding with this work was a renewed interest in the F1 engine as a "predeveloped" low-cost engine. Since the F1 met the above criteria, it was chosen as the CFD test case. The remainder of the period spent at MSFC was spent in producing a two phase CFD solution to the F1. Cells are to be chosen as input to the reaction reduction scheme from the solution.

3. F1 Solution

The physical parameters for the F1 were obtained from a recent review of the F1 testing. (Oefelelein and Yang, 1992) A two phase version(2.07) of Refleqs (CFDRC) was used. The code used allowed droplets to be introduced in up to 100 cells in the computational grid.

The grid chosen was 110 by 30, with the densest portion in the combustion chamber. (See figure 1.)

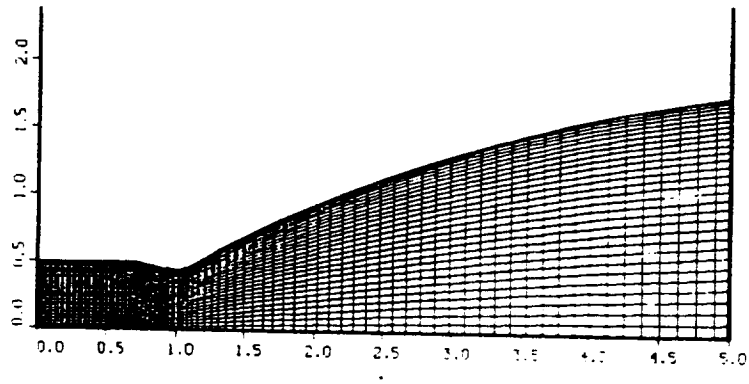

Figure 1. Computational grid used for the F1 engine.

Since the variation in mixture ratio needed to be modeled for testing of the reaction reduction scheme, an approximation of the complicated injector element location (Figure 2.) was included in the input file. Since the LOx had a 20 degree impingement angle and the RP-1 had a 15 degree impingement angle, the droplets were introduced into cells 2 and 3 respectively. Also the variation in orifice are per ring was also modeled to a certain extent, although the grid was not dense enough for a one-to-one correspondence with the injector rings. The presence of the baffles was ignored. A 3D solution would be required to take the presence of the radial baffles into account.

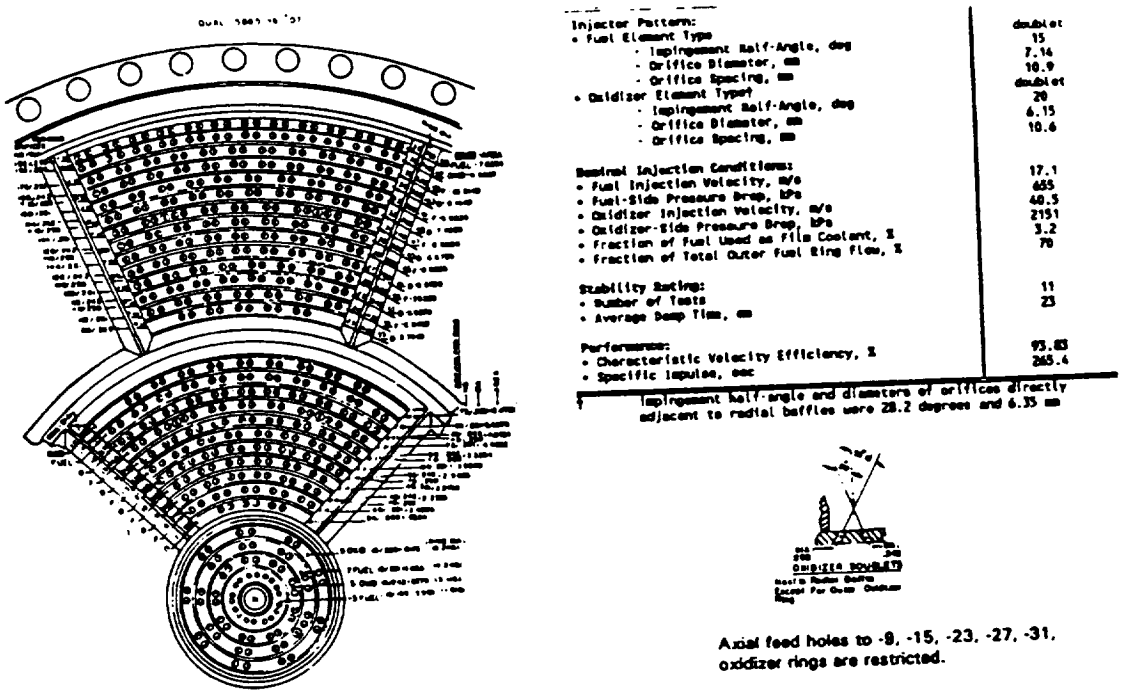

Figure 2. Injector configuration used in the CFD solution. (From Oefelein and Yang, 1992)

The inclusion of the variation of mixture ratio resulted in variation within the solution necessary to test the reaction reduction scheme. (Figure 3) However the actual test of the reduction procedure has yet to be performed due to time constraints.

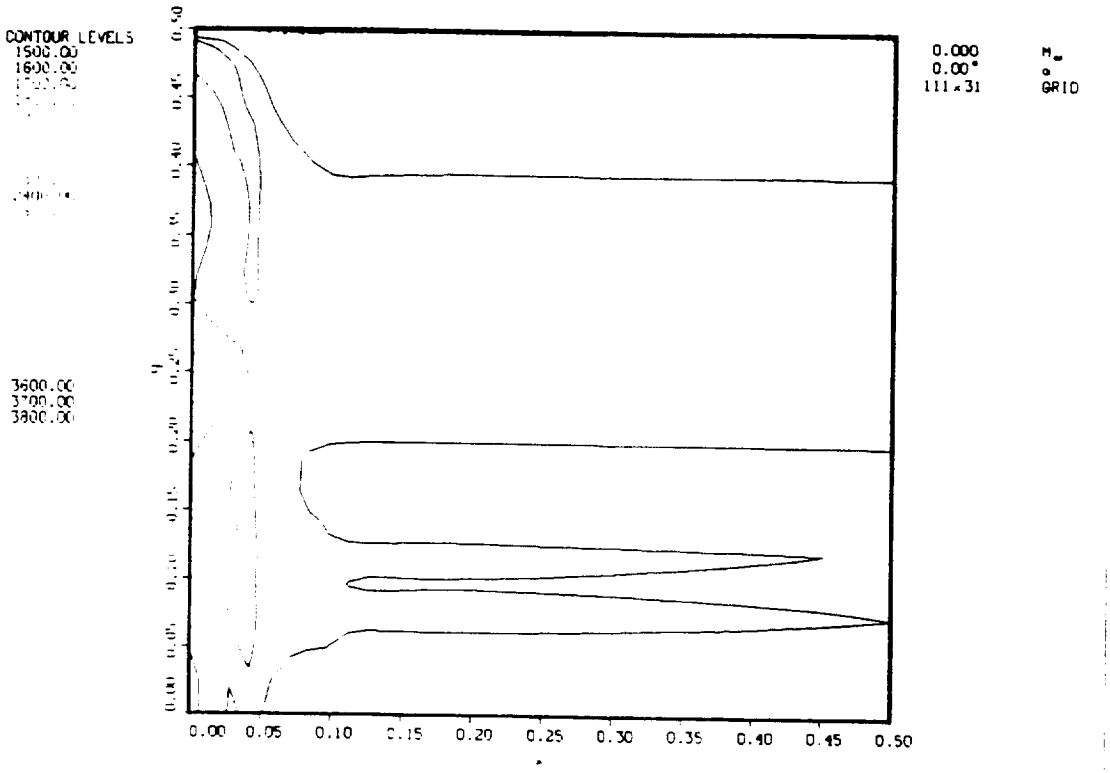

Figure 3. Temperature predictions near the injector.

4. Conclusions and Future Work

A two-phase solution of the FL engine with equilibrium in the vapor phase was found which showed enough variation within the combustion field to expect reduced reaction sets produced with the scheme previously outlined (Wikstrom, 1991) to vary with the computational grid.

The above conclusion has yet to be confirmed by implementation of the final CFD solution in the reaction reduction scheme. Selection of representative cells with the predicted inlet conditions is the next step in furthering this work.

A two-phase CFD code (Refleqs, CFDRC) can provide new insight as to the combustion within the F-1 engine. Better modeling of the impinging injectors should yield more meaningful results.

5. References

Oefelein, J.C. and Yang, V, "A Comprehensive Review of Liquid-Propellant Combustion Instabilities in F-1 Engines", Interim Version, July 23, 1992.

Wikstrom, C.V., "Computerized Reduction of Elementary Reaction Sets for Combustion Modeling", Final Report, ASEE/NASA Summer Faculty Fellowship Program, 1991.