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A Novel Approach for Modeling Chemical Reaction in Generalized Fluid System Simulation Program

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ABSTRACT

The Generalized Fluid System Simulation Program [1] (GFSSP) is a computer code developed at NASA Marshall Space Flight Center for analyzing steady state and transient flow rates, pressures, temperatures, and concentrations in a complex flow network. The code, which performs system level simulation, can handle compressible and incompressible flows as well as phase change and mixture thermodynamics. Thermodynamic and thermophysical property programs, GASP, WASP and GASPAK provide the necessary data for fluids such as helium, methane, neon, nitrogen, carbon monoxide, oxygen, argon, carbon dioxide, fluorine, hydrogen, water, a hydrogen, isobutane, butane, deuterium, ethane, ethylene, hydrogen sulfide, krypton, propane, xenon, several refrigerants, nitrogen trifluoride and ammonia. The program which was developed out of need for an easy to use system level simulation tool for complex flow networks, has been used for the following purposes to name a few: Space Shuttle Main Engine (SSME) High Pressure Oxidizer Turbopump Secondary Flow Circuits, Axial Thrust Balance of the Fastrac Engine Turbopump, Pressurized Propellant Feed System for the Propulsion Test Article at Stennis Space Center, X-34 Main Propulsion System, X-33 Reaction Control System and Thermal Protection System, and International Space Station Environmental Control and Life Support System design. There has been an increasing demand for implementing a combustion simulation capability into GFSSP in order to increase its system level simulation capability of a liquid rocket propulsion system starting from the propellant tanks up to the thruster nozzle for spacecraft as well as launch vehicles. The present work was undertaken for addressing this need. The chemical equilibrium equations derived from the second law of thermodynamics and the energy conservation equation derived from the first law of thermodynamics are solved simultaneously by a Newton-Raphson method. The numerical scheme was implemented as a User Subroutine in GFSSP.

A simple combustion model was developed for combustion of liquid hydrogen (LH_2) with liquid oxygen (LOX) using chemical equilibrium assumption. In this model it was assumed that H_2O, H_2, O_2, OH, H, and O were present in the products. The chemical equilibrium equations and the first law of thermodynamics were solved simultaneously by a novel computational method developed for determining the equilibrium composition and temperature of the combustion products. The modular FORTRAN code developed as a subroutine that can be incorporated into any flow network code with little effort has been successfully implemented in GFSSP as the preliminary runs indicate. The code provides capability of modeling the heat transfer rate to the coolants for parametric analysis in system design.

The current investigation considers the problem of combustion of LH_2 with LOX in a combustor with the assumption of H_2O, H_2, O_2, OH, H, and O constituting the products of combustion. We further assume that the products of combustion are in a state of chemical equilibrium. The schematic diagram of the problem is depicted in Figure 1.

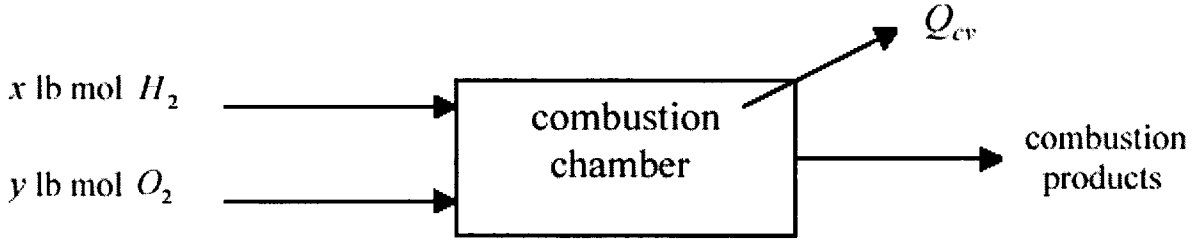

Figure 1: Schematic diagram of the combustion chamber.

For given inlet conditions and exit pressure, the resulting equations, which turn out to be coupled, non-linear, algebraic equations, are solved simultaneously. Three cases are considered; (a) stoichiometric case, (b) fuel rich case, and (c) oxygen rich case.

The chemistry mechanism used for the combustion process of liquid hydrogen with liquid oxygen is given by a set of reactions as follows

$$2H_2 + O_2 \Leftrightarrow 2H_2O$$
$$H_2 \Leftrightarrow 2H$$
$$O_2 \Leftrightarrow 2O$$
$$2H_2O \Leftrightarrow H_2 + 2OH$$

When the change in each species is considered, the overall reaction is written in terms of fractions, a, b, c, and d, that represent the rate of change of the number of moles in each reaction. This overall reaction can be expressed in terms of a, b, c, and d as follows

$$2H_2 + O_2 \rightarrow (2a-2d)H_2O + (2-2a-b+d)H_2 + (1-a-c)O_2$$
$$(2d)OH + (2b)H + (2c)O$$

Using the assumption of ideal gas mixture for the combustion products, the chemical equilibrium constants for the four reversible reactions were written in terms of a, b, c, and d. These yielded four equations in four unknowns. The mole fractions in terms of a, b, c, and d were also used in casting the energy equations in terms of these parameters. The thermodynamics properties in the equation (molar enthalpies of the species) were expressed as best-fit third and fourth order polynomial functions of temperature. Hence the fifth equation was obtained yielding five non-linear, coupled algebraic equations in five unknowns, namely a, b, c, d, and the temperature of the combustion products.

The resulting equations for the stoichiometric case are as follows

$$f_1 = \frac{(2a-2d)^2(3-a+b+c+d)}{(2-2a-b+d)^2(1-a-c)}\left(\frac{P}{P_o}\right)^{-1} - K_1 = 0 \qquad (1)$$

$$f_2 = \frac{(2b)^2}{(3-a+b+c+d)(2-2a-b+d)}\left(\frac{P}{P_o}\right) - K_2 = 0 \tag{2}$$

$$f_3 = \frac{(2c)^2}{(3-a+b+c+d)(1-a-c)}\left(\frac{P}{P_o}\right) - K_3 = 0 \tag{3}$$

$$f_4 = \frac{(2-2a-b+d)(2d)^2}{(2a-2d)^2(3-a+b+c+d)}\left(\frac{P}{P_o}\right) - K_4 = 0 \tag{4}$$

$$\begin{aligned} f_5 = {} & \dot{Q}_{c.v.} + (n_{H_2})_r(\Delta\bar{h}_{H_2})_r + (n_{O_2})_r(\Delta\bar{h}_{O_2})_r - (n_{H_2O})_p(\bar{h}^0_{f,H_2O} + \Delta\bar{h}_{O_2})_p \\ & - (n_{H_2})_p(\Delta\bar{h}_{H_2})_p - (n_{O_2})_p(\Delta\bar{h}_{O_2})_p - (n_{OH})_p(\bar{h}^0_{f,OH} + \Delta\bar{h}_{OH})_p \\ & - (n_H)_p(\bar{h}^0_{f,H} + \Delta\bar{h}_H)_p - (n_O)_p(\bar{h}^0_{f,O} + \Delta\bar{h}_O)_p = 0 \end{aligned} \tag{5}$$

The same procedure was used to obtain the corresponding five equations for the oxygen rich case and the fuel rich case so that the code could be used with any type of environment. The resulting system of equations in each case was similar. Newton-Raphson method was used in solving the resulting system of equations. In using this method, we developed subroutines to perform the tasks of Newton-Raphson solution in modular form. In this regard, subroutines were developed to enter generic residue equations, extract partial derivative terms numerically for forming the matrix of influence coefficients, and use Gaussian elimination method for solving a system of linear algebraic equations. This way, once the chemistry mechanism is chosen for any choice of propellants, the residue equations resulting from the equilibrium constants and the conservation of energy principle can be entered through the equations subroutine and the rest of the modular code does not have to be modified. It was shown that the Newton-Raphson method provides a stable numerical solution method with a single initial guess yielding solutions for up to 15 percent oxygen rich and 15 percent fuel rich cases. The computer calculations were compared against hand calculations using linear interpolation for the enthalpies and for the chemical equilibrium constants for sample problems. The results obtained were very close, validating the accuracy of the numerical solution.

The modular code developed was integrated into GFSSP and run for several case studies. These preliminary runs showed that the integration of the modular code was successful. The authors are currently conducting more runs for establishing a scheme for determining a good initial guess that will yield a stable solution over the entire range of applicability.

References

[1]Majumdar, A. (1999), "Generalized Fluid System Simulation Program (GFSSP) Version 3.0", Sverdrup Technology Report No. MG-99-290, Contract No. NAS8-40836.