THERMOCHEMICAL EXPLORATION OF SUPERSONIC REACTING FLOWS OF A TYPICAL SCRAMJET ENGINE CONFIGURATION USING OPEN SOURCE CFD CODE OPENFOAM

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ABSTRACT

In this study the characteristics of mixing and reaction between hydrogen and air is studied within a supersonic combustor using the open source code, OpenFOAM. Characteristics of turbulent mixing of hydrogen and air in an inert environment and turbulent combustion of hydrogen and vitiated air are studied. Various turbulence models are used and compared in the study. For simulation chemical reactions single step Eddy Dissipation Concept and Partially Stirred Reactor with detailed chemistry are used. The exit profiles from the various models are compared amongst themselves and also with experimental data.

Keywords: OpenFOAM, Eddy Dissipation Concept, Partially Stirred Reactor, Scramjet, Reacting Flows

INTRODUCTION

The conventional air breathing engines such as the gas turbine or the turbojets are limited in their ability to operate at speeds higher than Mach 5 due to their drastic drop in efficiency as the speed increases. This problem arises because of the fact that these engines use up a large amount of energy produced by the fuel to run the mechanical components within the engine such as compressor, fan etc. This limitation has led to the development of an alternative method of propulsion which is capable of achieving sustained flight at hypersonic speeds.

Two such engines which fall in the aforementioned category are the ramjet and scramjet. Both these engines are air breathing engines with minimal or zero moving parts and are designed for sustained high speed flights.

The ramjet and scramjet both utilise their geometry to form compression waves near the inlet of the engine which convert the high speed of air near the inlet into high pressure and high temperature which are favourable for combustion of fuel. The energy released from the burnt fuel is converted into thrust using a nozzle section behind the combustor. The primary difference between a ramjet and scramjet is that combustion within a scramjet takes place at supersonic speeds.

The combustion in a scramjet is characterized by very high velocity of air flow within the combustor. This lead to very low residence time of air inside the combustor.Because of low residence time, adequate mixing of air and fuel must takes place before the mixture enters in the combustor.

In order to achieve this, various numerical and experimental researches Are being carried out to understand the complex flow field within a scramjet. In this study, the use of the open source software OpenFOAM in the field of supersonic reacting flows is investigated. The results obtained from the software are compared with the results obtained from the experiment carried out by Marshall C. Burrows and Antole P. Kurkov. The results are analysed to understand the deviation from real data and the reason for its occurrence..[1], [2]

METHODOLOGY

Experimental details

In order to design supersonic combustors numerically, experimental data on the diffusive mixing and reaction of fuel and air at very high temperatures, which are characteristics of high speed flight at around Mach 6, is needed.

In this section, the schematic and the experimental details of the Burrows and Kurkov setup (**Fig.1**) is explained. The results from this experiment are used to compare the results from numerically simulated cases.

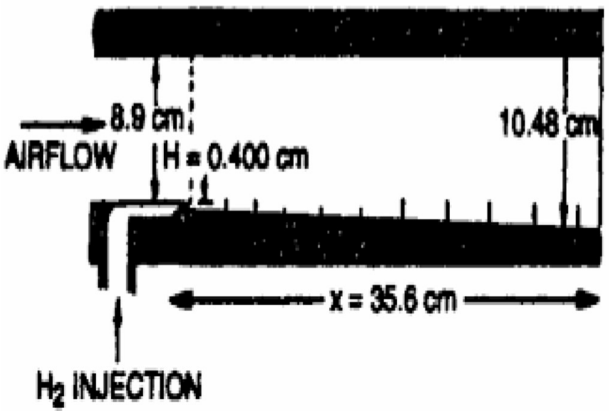

FIGURE 1: SCHEMATIC DIAGRAM OF THE EXPERIMENTAL SETUP

In computation, on the left side of the combustor an extra length of about 0.5 m (not shown in the schematic) is given for the incoming air to develop a boundary layer as it enters the combustor from the facility nozzle. The inlet of combustor is having a cross-section of 51 mm × 89 mm. The air from the

facility nozzle enters the combustor at a velocity of Mach 2.44 with a static temperature of 1270 K and a static pressure of 1 atmosphere. At the end of the facility nozzle and the start of the combustor, hydrogen was injected using a slot injector of thickness 0.76 mm sitting on top of a 4 mm step. After the injector the test section diverged to an area of 51 mm x 104.8 mm giving it a divergence angle of 1.78°. The length of the combustor from the fuel injector to the outlet of the combustor is 356 mm. A provision was given to regulate the temperature of inlet hydrogen gas between 300 K and 800 K. The properties of vitiated air and hydrogen used for the experiment are listed in specially designed water-cooled, wedge-shaped thermocouple probes were used to measure temperature along the exit of the combustor. The exit temperatures were reproduced with an accuracy of ±3%. A similar water-cooled probe was used for pitot pressure measurements with an accuracy of ± 2.5% except in the reaction zone, where measurement varied over a wider range from run to run. Gas sampling analysis was reported to be accurate within ±2.0%. The sampling probes were also used as cooled gas pyrometers to indirectly measure the stream total temperature

Parameters	Vitiated Air		Hydrogen
	Mixing Case	Reacting Case	
Mach No.	2.44	2.44	1.0
Total Temperature (K)	2276	2380	303
Total Pressure (bar)	18.5	17.1	1.85
Mole Fraction Composition			
X_{H_2}	0.0	0	1.0
X_{H_2O}	0.322	0.373	0.0
X_{O_2}	0.0	0.199	0.0
X_{N_2}	0.678	0.428	0.0

TABLE 1: PROPERTIES OF VITIATED AIR AND HYDROGEN

Water cooled probes were used to obtain gas samples at the exit of the combustor. The probes were designed to trap gas samples leaving the combustor which were later analyzed using a mass spectrometer. Instrumentation probes were provided which were moved along the exit in succeeding runs in order to obtain an exit profile of the parameters in the exit section. Most of the measurements were made within 40 mm distance from the lower wall. Four windows were mounted flush within the combustor wall in order to make visual inspections and photographic observations. The ignition delay were observed from the photographs of OH radiation.

Computational Methodology

The numerical simulations were carried out in the open source software OpenFOAM which solves the continuity of mass, momentum (3-D Navier-Stokes) and energy equations. To simulate high Mach number compressible reacting flow, a density based solver, rhoReactingFoam, was used.

The flow at high speeds is inherently turbulent due to its high Reynold's number. Because of its turbulent nature, it is vital to incorporate turbulence modelling into the numerical simulation. Various two equation turbulence models were used namely, realizable k-ε and k- to determine their predictive capability in turbulent reacting flows.

Combustion Modelling

There are various methods available to model the chemistry of H_2- air combustion in OpenFOAM. The simplest of these all is the laminar combustion in which the solver simply assumes that the combustion proceeds at a rate decided by the reaction rate. This yields reasonably good results with very less computational effort.

The next method, the Eddy Dissipation Concept, predicts combustion based on the assumption that the reaction rate of a reaction in case of turbulent flow with diffusion flames is determined by the rate of mixing of the two species in very small scale regions called fine structures. This theory utilizes the assumption that in turbulent flow, the energy from the large eddies is passed down to smaller eddies with release of energy each time the energy is passed. This process continues down to a level where the complete turbulent energy is released as heat energy in very small regions. These regions where the turbulent energy is totally dissipated into heat energy are called fine structures. The mean reaction rate given by EDC is. [3].

$$\tilde{\omega}_i = \frac{\gamma^2 \chi}{\tau^*} (Y_i^\circ - Y_i^*)$$

Where χ is the fraction of the fine structures where reaction occurs. The superscripts '°' and '*' refer to the surrounding fluid and fine structure regions respectively.

The next model utilised was the Partially Stirred Reactor abbreviated as PaSR. The PaSR is based on the use of Probability Density Functions to predict the rate of reaction in a fine structure whilst assuming homogeneity in it. In PaSR, the reacting cell is split into two zones, a reacting zone and a non-reacting zone. The reacting zone is modelled as a Perfect Stirred Reactor (PSR) where all the reactants are assumed to be perfectly mixed with each other. The first considers the change of concentration from unburnt gases to burnt gases. The second one considers the turbulent mixing of burnt gases with oncoming fresh reactants. The reaction rate in PaSR is directly proportional to the chemical reaction time to the total conversion time in the reactor [4].

$$\kappa_k = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

τ_{mix}

Where τ_c is the time taken for the reaction in the cell and is the time taken for the reacted mixture to get mixed up with the non-reacted mixture.

Chemistry Modelling

There are three different types of chemistries mainly used for modelling combustion between hydrogen and air. Single step, seven step and twenty seven step reaction mechanisms are used in the simulations. The single step reaction is the most simple and least computationally expensive but the results are further off from the experimental data as compared to the seven step and the twenty seven step mechanisms. However, the greater, the number of steps in the detailed chemistry, the

requirement of computational power is more; hence it is important to tradeoff between the two to optimize and obtain the required accuracy of results.

RESULTS AND DISCUSSION

The qualitative features of mixing of hydrogen and air without any reaction within the combustor can be observed in the contours below. Fig.2 shows that the inlet of hydrogen into the combustor causes the generation of a shockwave which hits the upper wall at approximately 210 mm from the injector. The hydrogen stream for the most part adheres to the reactor's bottom wall and diffuses to a thickness of around 25 mm at the reactor exit. Various turbulence models were studied but the best results were obtained from the *realisable k-ε model*. The computed pitot pressure at the exit of the combustor was compared with the experimental value and good agreement was found between the two. Fig.2 shows the pressure contour of turbulent mixing of hydrogen and Fig.3 shows the mole fraction contour of hydrogen for the same case. Figs. 4, 5 and 6 show the variation of water, nitrogen and hydrogen mole fractions in the turbulent mixing case with different turbulence models alongwith experiment

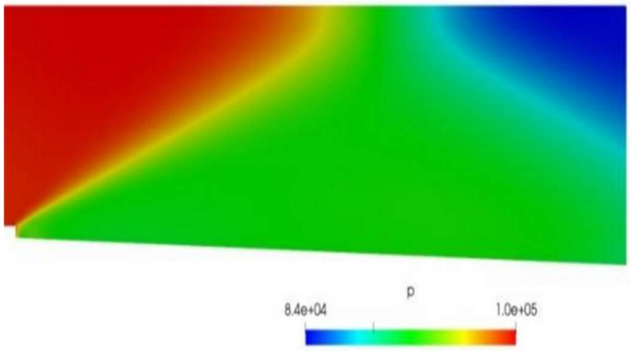

FIGURE 1: TURBULENT MIXING PRSUURE CONTOUR.

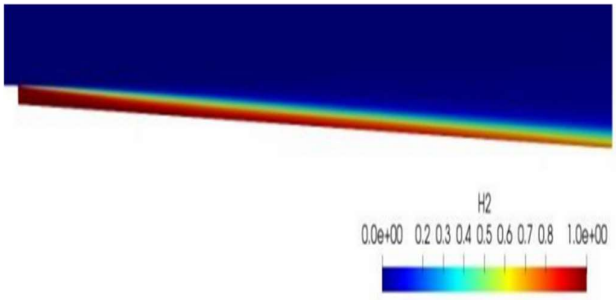

FIGURE 3: TURBULENT MIXING H_2 CONTOUR

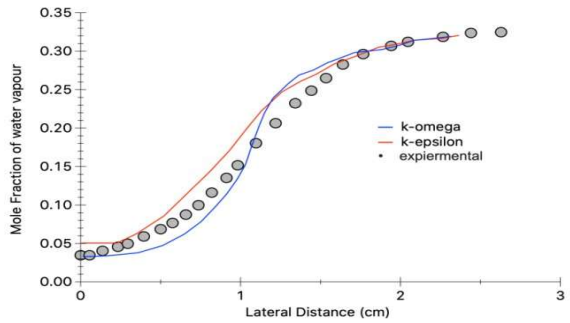

FIGURE 4: COMPARISON OF H_2O EXIT PROFILES WITH DIFFERENT TURBULENCE MODELS

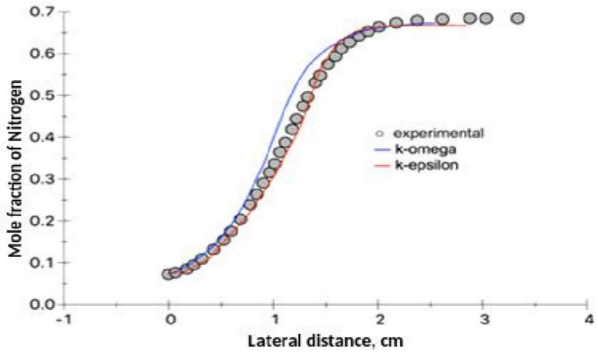

FIGURE 5: COMAPARISON OF N_2 EXIT PROFILES

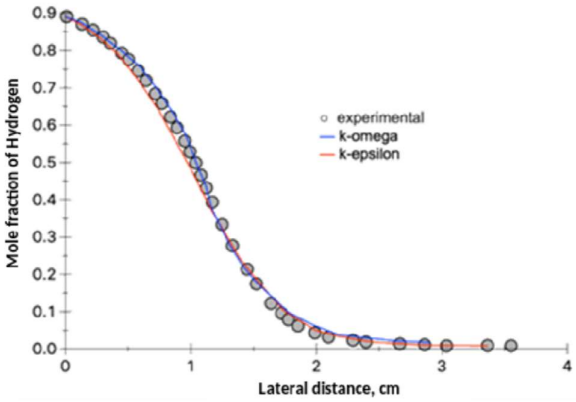

FIGURE 6: COMPARISON OF H_2 EXIT PROFILES

The results are not an exact match with the experimental data but there is reasonably good agreement between the two as can be seen from the exit profile plots of the various species.

For simulation of the reacting case, the maximum temperatures were best predicted by the EDC model but the best match of the contours was obtained by PaSR model. The case was also run using singlestep simple chemistry, and 7 and, 27 steps detailed mechanisms. The comparisons of H_2O mole fraction is shown in Figs.7 for different chemistries. Figs.8, 9 and 10 show the variation of mole fractions of, and with various turbulence models. While single step chemistry resulted in almost instantaneous combustion of hydrogen as it is introduced into the combustor, the lag in combustion is best predicted by the 27 step chemistry. Also, in the EDC model, the peak temperatures at the exit of the combustor occurs at 10 mm from the bottom wall whereas in the experimental case this occurs at 20 cm from the bottom wall. In the PaSR, however, the peak temperature profile is in fair agreement with the experimental data. Overall, the 7 step detailed chemistry combined with the PaSR model predicts the best results of all cases. Fig.11 shows the temperature contour obtained by the PaSR model with the seven step detailed chemistry. Figs. 12 to 17 show the various contours obtained in the turbulent reaction (realizable k-epsilon) with 27 step chemistry. All simulations in the matrix are well converged and a sample residual plot for the case with PaSR combustion model and 7 step 7 species chemical mechanism is given in Fig. 18, minimum 5 decade fall is ensured in residuals apart from 1% flux balance error limit.

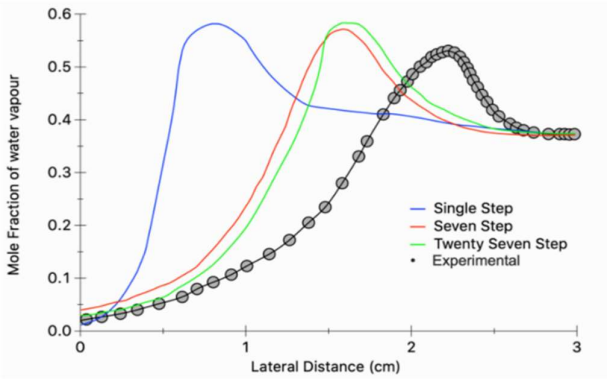

FIGURE 7: COMPARISON OF WATER MOLE FRACTION AT EXIT WITH DIFFERENT CHEMISTRIES.

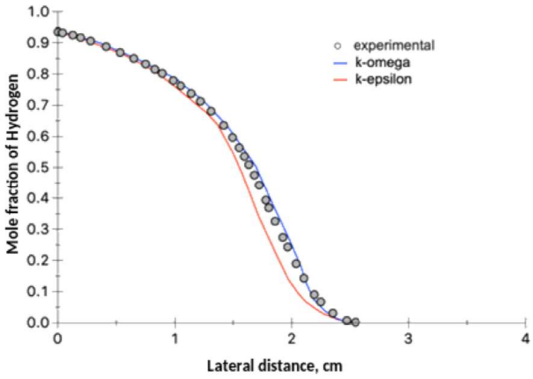

FIGURE 8: COMPARISON OF H_2 MOLE FRACTION.

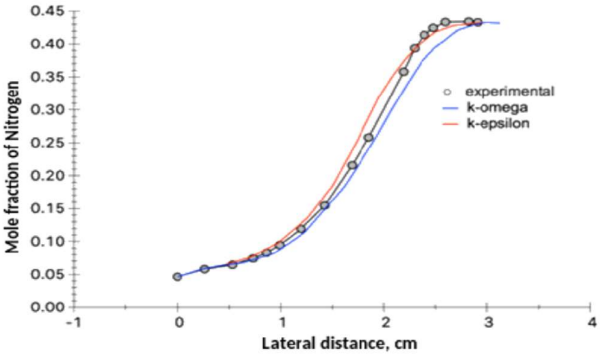

FIGURE 9: COMPARISON OF N_2 MOLE FRACTION.

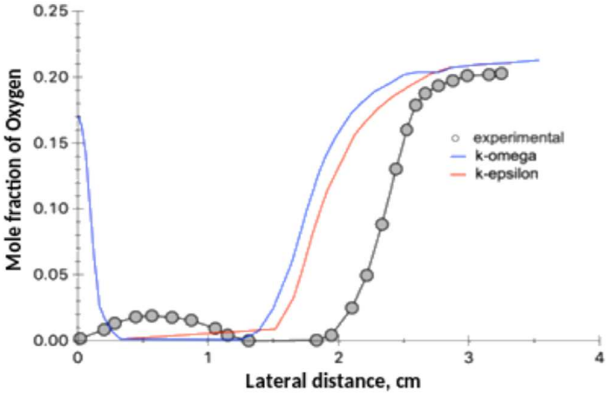

FIGURE 10: COMPARISON OF O_2 MOLE FRACTION

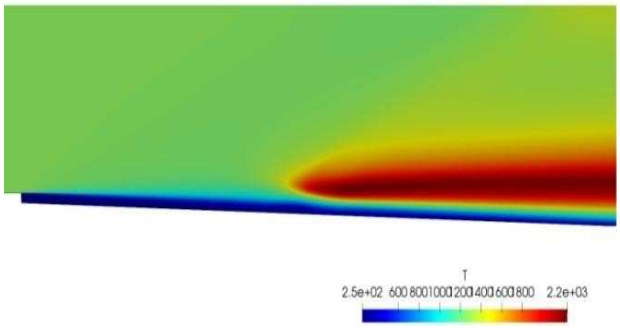

FIGURE 11: TEMP. CONTOUR OF REACTING CASE (7 STEP CHEM.)

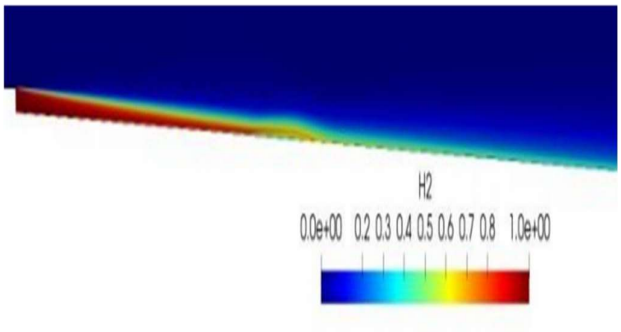

FIGURE 12: H2 CONTOUR OF REACTING CASE (27STEP CHEM.)

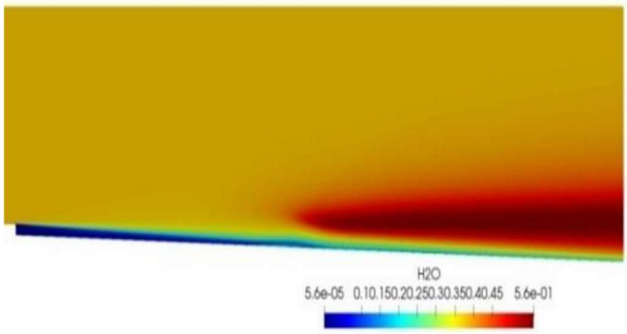

FIGURE 13: H2O CONTOUR OF REACTING CASE (27 STEP CHEM.)

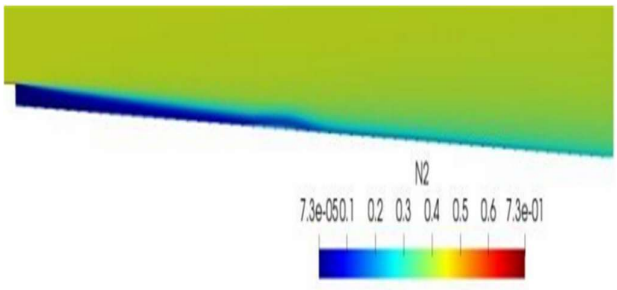

FIGURE 14: N2 CONTOUR OF REACTING CASE (27 STEP CHEM.)

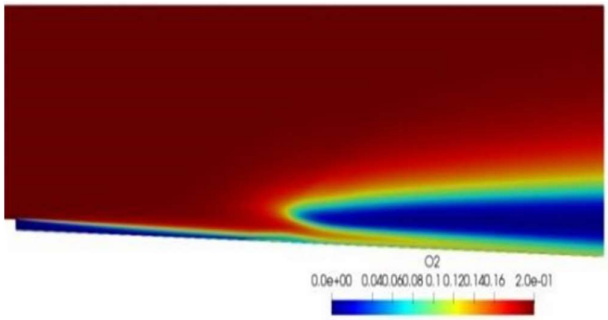

FIGURE 15: O2 CONTOUR OF REACTING CASE (27 STEP CHEM)

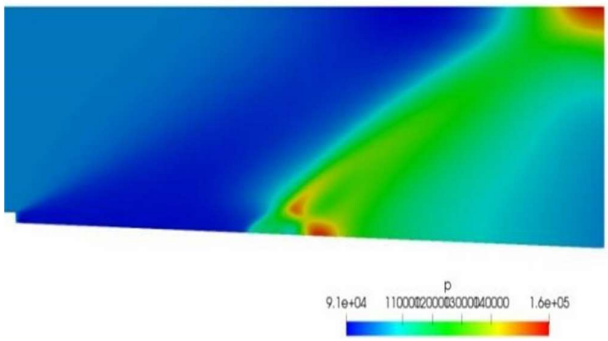

FIGURE 16: PREASSURE CONTOUR (27 STEP CHEM)

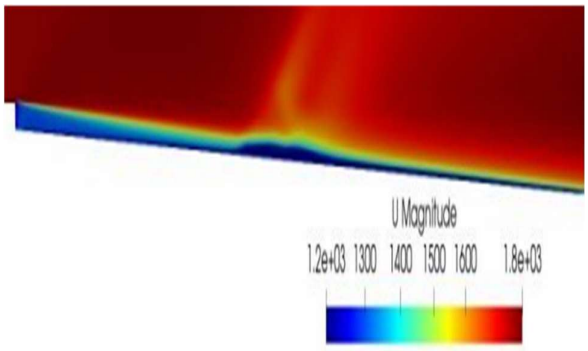

FIGURE 17: VELOCITY CONTOUR (27 STEP CHEM)

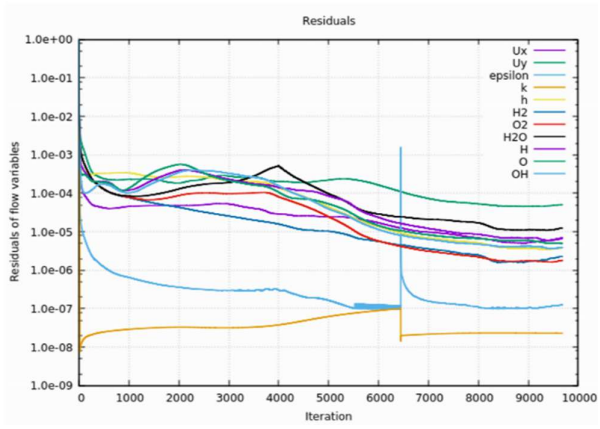

FIGURE 18: RESIDUALS PLOT FOR A SIMULATION CASE.

CONCLUSIONS

While extensive work is yet to be carried out in the field of hypersonics, there has been considerable progress. With further funding being invested into this field, there is an increased demand for more accurate predictive models for supersonic reacting flows. While commercial codes offer the solutions to some extent, openfoam gives the user the flexibility to play around with the source code and change the solvers. This leads to an increased scope of quicker and more focussed development taking place in the required field. As shown in the results above, the native solvers themselves are providing fairly accurate results.

ACKNOWLEDGEMENTS

This research was supported by the Defence Research and Development Laboratory, Hyderabad. We would like to thank the Department of Computational Dynamics and Dr. Debasis Chakraborty for providing us with the computational power required to perform these computational calculations. We would also like to thank all the scientists and staff who directly and indirectly contributed in bringing out this paper.

REFERENCES

[1] H. G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, computers in physics, vol. 12, no. 6, nov/Dec 1998

[2] Burrows, M.C. & Kurkov, A.P. Analytical and experimental study of supersonic combustion of hydrogen in vitiated air stream. Report No. NASA-TMX-2828, 1973.

[3] Gran, I R. Mathematical modeling and numerical simulation of chemical kinetics in turbulent combustion. PhD Thesis, university of Trondheim, the Norwegian institute of technology, 1994.

[4] Amit Bhave and Markus Kraft. Partially Stirred Reactor Model: Analytical Solutions and Numerical Convergence Study of a PDF/Monte Carlo Method.