ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

Computational Fluid Dynamic Analysis Of Combustion In Two Dimensional Star Shaped Perforation And Circular Perforation Ammonium Perchlorate Composite Propellant With HTPB Binder

K.M. Pandey[1] and Sunita Deb[2]

[1]Professor, Department of Mechanical Engineering
National Institute of Technology, Mechanical Engineering, Assam, Silchar, 788010, India
E-mail ID: kmpandey2001@yahoo.com
[2]M.Tech Scholar (Thermal Engineering), Mechanical Engineering
National Institute of Technology, Mechanical Engineering, Assam, Silchar, 788010, India
E-mail ID: sunitadeb89@gmail.com

Abstract: - Solid propellants are used in forms called grains. A grain is any individual particle of propellant regardless of the size or shape. The shape and size of a propellant grain determines the burn time, amount of gas and rate produced from the burning propellant and consequently thrust vs time profile. In this paper, the difference in the combustion temperature obtained and velocity magnitude of ammonium perchlorate propellant with (Hydroxyl Terminated Poly Butadiene) HTPB binder for circular perforation and five leg star shaped perforation has been brought out with the help of Computational Fluid Dynamics (CFD) software.

Keywords: - Composite Propellant**,** Computational Fluid Dynamics, Eddy Dissipation

INTRODUCTION

Rocket propellant is a material used by a rocket as, or to produce in a chemical reaction, the reaction mass (propulsive mass) that is ejected, typically with very high speed, from a rocket engine to produce thrust. Chemical rocket propellants undergo exothermic chemical reactions to produce hot gas. There may be a single propellant, or multiple propellants; in the latter case one can distinguish fuel and oxidizer. The gases produced expand and push on a nozzle, which accelerates them until they rush out of the back of the rocket at extremely high speed. They can be basically classified into two types, liquid propellants and solid propellants. The burning of solid propellants based on physical mixtures of a solid oxidant and a solid fuel has been the subject of a number of attempts to devise a theoretical model for the mechanism of the process which determines the linear burning rate and its variation with parameters such as combustion pressure, component particle size, initial temperature and composition. Solid propellants can be further classified into double base propellant and composite propellant. Double base propellants contain two major ingredients; nitro glycerine and nitro cellulose. Composite propellants are a mixture of finely ground oxidizer, commonly ammonium perchlorate (AP) fuel, generally aluminum, and a binder like HTPB (hydroxyl terminated polybutadiene). Composite propellants have a higher combustion

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

temperature and a higher performance than double base propellants. Grain is an essential area in the study of solid propellant. The shape of the grain determines the surface area of the combustion and thus determines the amount of gases that are produced to propel the rocket. The physiochemical processes that occur during the combustion of AP-HTPB propellant include condensed-phase heating, degradation of AP and HTPB, melting and surface pyrolysis, and gas-phase reactions. The flame structures and burning behavior depend on several factors, such as propellant composition, AP grain size, initial and ambient conditions, and propellant morphological configuration. Many works have been carried out experimentally to find out the effect of pressure dependence of burn rate, effect of particle size etc. Theoretical numerical modeling has also been done. The effect of turbulence has been considered. Steady-state solution (with all the unsteady fluctuations averaged out) is desired rather than a detailed time-accurate one that captures every little vortex. As a result, there are unsteady (turbulent) motions affecting the flow that cannot be resolved directly. The flow must therefore be modeled. There are various turbulence models. Turbulence models are generally classified according to which governing equations they apply to (e.g. Reynolds-averaged Navier-Stokes or Large Eddy Simulation equations). Within these broader categories, they are further broken down by the number of additional transport equations which one must solve in order to compute the model contributions. Algebraic (Zero-Equation) Models are the simplest (and least computationally expensive) models are the algebraic models. These are also called "zero-equation" models, because they do not solve an additional transport equation in order to predict the contributions of the turbulence. These models are not very general, so they are not used much anymore, but when they can be applied, they often give very good results. One-Equation Models are one level up in the turbulence modeling hierarchy are the one-equation models. These solve a single transport equation for a quantity which is used to obtain the turbulent viscosity. Currently, the most popular one-equation model is the Spalart-Allmaras model. This model has been shown to give acceptable results for a wide variety of situations and is known for its stability. Other one-equation models that are available in production codes include the Baldwin-Barth model and the Goldberg pointwise model. An advantage of the Goldberg model is that is does not require the calculation of the distance from each field point to the nearest wall. This makes it easier to implement than many other models. On the other hand, its results are often not as good as from the Spalart model (which does require a wall distance calculation). Two-Equation Models require the solution of two additional governing equations in order to compute the contributions of turbulence to the mean flow. Along with the Spalart-Allmaras model, two-equation models make up the bulk of the turbulence models used for production CFD. Two of the most common models are the Menter SST model and the k-epsilon model, but there are many others (too numerous to mention). The SST model is a blend of a k-omega model, which is used near walls, and a k-epsilon model, which is used in regions far from walls. This model is fairly robust and

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

generally does a good job near solid boundaries. It also is often found to do a better job at capturing recirculation regions than other models. The k-epsilon model would more properly be called a family of models. Specialized version have been developed for so many specific flow configurations that there are now almost as many different k-epsilon models as there are CFD practitioners trying to use them. Some of the more common variants include the Jones-Launder, Chien, and RNG k-epsilon models. More recently, as greater computer resources have become available, there has been a renewed effort to look at modeling the Reynolds stresses directly instead of reducing the all effects of turbulent eddies to a turbulent viscosity term. As a result, there are now several variations of Reynolds stress models and algebraic stress models available in major CFD codes. These models are often quite computationally expensive, compared to a conventional one- or two-equation model, but under the right flow conditions, they have been shown to provide improved results.

LITERATURE REVIEW

Laredo and Gany [1] studied the surface phenomenon associated with the combustion of highly metalized (40 – 50 % Boron) solid propellants by means of high speed photography using a windowed frame burner strand. They found out that propellants containing boron additives in the range of 40 – 50 % show irregular burning with some periodic phenomenon concerning the regression rate metal agglomeration and ejection of unburnt propellant layers. They also studied the effects of pressure on the combustion phenomenon. They observed the increase of agglomerate size above a pressure of 50 bar.

Ajaz [2] in 1995 conducted experiments to determine the percentage of Aluminium in HTPB based composite propellants. He found that in pastes containing aluminum (Al) it is important to eliminate the entire Al before starting the actual reaction (distillation). The results obtained are in the range of + 0.05% for pastes with and without Al whereas the range is +0.02% for pure AP.

Kishore and Sridhara [3] in 1996 were the first one to report the influence of Polymeric binders on the combustion behavior of ammonium perchlorate Composite Propellants. In admixture with ammonium perchlorate (AP), dicarboxylic acids were used to simulate the commonly used telechelic polymers such as carboxy-terminated polybutadiene (CTPB) fuels. They showed that the burning rates r vary exponentially with M, the molecular weight of the acids. The dependence of r, at constant pressure and initial temperature T0, on M of a fuel may be called the 'molecular weight sensitivity of the burning rate', expressed as

$$\sigma = (\delta \ln r / \delta M)P, T0$$

Where σ is the fractional change in r per gmol of the -(CH2)- unit. The value of σ seems to depend strongly on the chemical structure of the backbone and is closely related to the combustion mechanism of the constituent fuel in the condensed and gas phases. They have also shown that the volatilization rate decreases with increase in M, but the ratio of

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

the condensed-phase to gas-phase heat release increases with M.

Thakre and Young [4] described the properties of solid propellant like high specific impulse, high densities etc. They also described the combustion characteristics of solid propellants. They took the example of a steady state self deflagrating monopropellant RDX strand which resembles the combustion of solid propellant in a laminar premixed flame. The combustion wave structure was divided into three layers that are solid phase, subsurface and gas phase. The propulsive performance depends upon the characteristics.

Harthi and Williams [5] in 1998 studied the effects of fuel binder and oxidizer particle diameter on the combustion of ammonium perchlorate based propellants. The burning rate was observed to vary as a function of fuel concentration. They found that the contribution of the heat produced by the condensed phase reactions to the total heat released was greater for the AP/ paraffin mixtures. Based on the results obtained, they proposed a reaction mechanism for the decomposition of the Ammonium perchlorate composite propellant and its combustion process.

Fitzgerald and Brewstar [6] in 2004 conducted experiments to study the combustion behavior of 2D laminar propellants. They found that the flame-surface structure is a function of length scale (in this case, fuel-layer thickness), pressure, and equivalence-ratio disparity between the non premixed fuel and the oxidizer regions (binder-matrix equivalence ratio).

Boldyrev [7] in the year 2006 described the thermal decomposition and thermal stability of Ammonium perchlorate. The rate of thermal decomposition sharply decreases at the moment of phase transition because rearrangement of the lattice from the rhombic into cubic at the moment of transition results in sharp worsening of the conditions for the accumulation of products catalyzing thermal decomposition in the system. Properties of ammonium perchlorate has also been discussed which includes dislocations in Ammonium perchlorate, conductivity of ammonium perchlorate etc. The products of decomposition depend upon the temperature. At about 300 ^{o} C, Cl_2, O_2, N_2O, H_2O are formed. Above 380 ^{o} C, N_2O is formed instead of N_2. Further investigations are required on the exact decomposition reactions although a lot of work has been carried out in this paper.

Favale and Miccio [8] in 2008 modeled unsteady and perturbed combustion of heterogeneous composite propellants. Their work included a better simulation of the Naviers Stokes Equation coupled with species conservation mass balance and energy conservation equations. The model is also able to simulate the process under the action of an external perturbation, which is produced by a time-dependent heat flux impinging the propellant surface (e.g. laser source).

Cai et al [9] devised a comprehensive theoretical numerical model for treating

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

AP/HTPB composite-propellant combustion in a rocket-motor environment. The combustion processes which comprise of gas phase and condensed phase are coupled at the surface to determine the propellant burning behavior.

S.N. Jawalkar et al [10] in 2009 prepared different composite propellant mixtures using ammonium perchlorate, aluminum powder and hydroxyl terminated polybutadiene by varying the percentage of plasticiser and addition of toluene diisocyanate at different temperatures. They studied their different properties such as viscosity build-up, mechanical and ballistic properties and sensitivity. The results they obtained showed that on decreasing the plasticiser content, there is a significant enhancement in end of mix viscosity, tensile strength and modulus while elongation decreases drastically while the sensitivity increases accordingly.

Gross and Beckstead [11] in 2010 studied the complexities of the flame structure above a composite propellant containing 86% ammonium perchlorate (AP) and 14% hydroxy-terminated-polybutadiene (HTPB) using a two dimensional, detailed gas-phase kinetic mechanism diffusion flame model. With the help of numerical model they could predict three combustion zones according to the particle size.

Xiong Gang Wo et al [12] in 2011 studied the burning rates of different composite modified double base propellants (CMDB) at different pressures. They found that for higher pressure ranges, 15 – 22 MPa, the burn rate of blank propellant is lower than the metalized propellants but in the lower pressure ranges, 1- 15 Mpa, the burn rate of the blank propellant is higher than that of the metalized propellant. The role of the metal nature in agglomerate formation has been shown. The use of magnesium demonstrated a significant decrease in the formation of unburnt metals and an increase in the metal oxide. Besides by using nickel, the carbon content of the residues decreased along with the agglomerate size. For nickel CMDB, there is a large amount of unburnt nickel in the residues.

Vandenkerckhove and Jaumotte [13] studied the burning mechanism and erosive burning of Ammonium perchlorate Propellants. They observed that for coarse granulations and low oxidizer contents, the burning rate is higher at low pressure and smaller at high pressure than that of pure perchlorate. For fine granulations and high oxidizer contents, the burning rate is higher at all pressures in the considered range. For coarse granulations and low oxidizer contents, the burning rate is higher at low pressure and smaller at high pressure than that of pure perchlorate. For fine granulations and high oxidizer contents, the burning rate is higher at all pressures in the considered range. On the other hand, in the high pressure range above 60 kg/cm^2, it seems dubious that the main diffusion flame still plays a significant role in transferring heat to the surface because otherwise the propellant burning rate would be consistently higher.

J. Powling [14] conducted experiments relating to the combustion of Ammonium perchlorate based propellants. He observed a distinct variation of surface temperature,

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

when gaseous fuel at low temperature was used. The rate of flame travel down single binder/ammonium perchlorate interfaces have been measured as a function of pressure. Through his experiments he showed that the dissociation of Ammonium perchlorate is generally represented by a kinetic decomposition law than by equilibrium law. He found that at low pressures, the burning rates of composite mixtures of ammonium perchlorate with organic fuels are little affected by fuel-binder properties, other than heat of combustion, but at high pressures the converse is true.

MODELING OF THE STAR SHAPE PERFORATION AND CIRCULAR PERFORATION IN PROPELLANT GRAIN

Two cases have been considered to find out the effect of the combustion area of the propellant. One is propellant with circular perforation and the other one is five leged star shaped perforation better known as five star configuration. Two dimensional modeling is done for both the cases. The geometry of these have been modeled using modeling and meshing software. The outer radius of the circular perforation is taken to be 0.006 mm the five star configuration is specified as outer radius 0.031 mm and inner radius 0.006 mm. The mesh information of both the models are given below.

Five star configuration :

Cells	Faces	Nodes	Partitions
1936	4114	2178	1

Circular configuration:

Cells	Faces	Nodes	Partitions
787	1611	824	1

The inlet area of the star shaped perforation is 0.26383679 m^2 and the inlet area of the circular perforation is 2.872e-05 m^2.

COMBUSTION MODELING

Combustion process in a solid propellant is complex process. The physicochemical processes that occur during combustion comprise of condensed phase reactions, degradation of ammonium perchlorate, melting, surface pyrolysis and gas phase reactions. Therefore it becomes extremely complicated to model these reactions using numerical models. Therefore a one reaction model has been considered which has been developed by Cai et al., to have a comprehensive numerical model to for treating AP-HTPB composite-propellant combustion in a rocket-motor environment**.** Ammonium perchlorate is the oxidizer which evolves gases like O_2, N_2O etc which are oxidizers. The binder HTPB also acts as a fuel which releases C_2H_4 at high temperatures.

One chemical reaction is considered for the total combustion process. The effect of turbulence has been taken into account which was not taken by Cai et al. Turbulence mixes the gaseous species involved in the reaction.

The one step chemical equation [7] that was developed is as follows:

$$1.617\ H_2O + 1.105\ O_2 + 0.261\ N_2 + 0.118\ N_2O + 0.229NO + 0.75\ HCl + 0.1149\ Cl_2 + 0.5229\ C_2H_4 \longrightarrow 0.4686\ CO +$$

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

$0.5773\ CO_2 + 0.0999\ Cl + 0.038\ H + 0.8799\ HCl + 0.2365\ H_2 + 2.27H_2O + 0.479N_2 + 0.0289\ NO + 0.0133\ O + 0.1394\ OH + 0.0499\ O_2$

The reactants are at an initial temperature of 300 K and pressure of 69 atm. The reactants are considered to be released from the legs of the star in case of star shaped perforation or in the case of circular perforation, from the outer circumference. The reaction gives out products which then flow towards the inner circumference.

Mass flow rate has been considered to be constant at 10.3224 kg/m^2sec for both the cases as the surface is assumed to be non regressing. The thermal conductivity, and dynamic viscosity of the individual species constituting the gaseous mixture is assumed to be non variant as these properties change a little in gaseous phase at very high temperature.

For turbulence modeling, standard k-ϵ turbulence was used with viscous heating. The reaction is assumed to be taking place at the surface of the propellant and after combustion the gases move towards the centre of the combustion zone from the periphery of the surface. Eddy dissipation model is chosen as it incorporates the effects of turbulent mixing of the reactants.

RESULTS AND DISCUSSIONS

Temperature and velocity contours have been obtained assuming that the burning surface is constant for both circular and star shaped perforation. Figure 1 shows the static temperature contour of the five star configuration and Figure 2 shows the static temperature contour for the circular perforation. From the figures it is clear that for five star configuration, the highest temperature obtained after combustion is about 3370 K whereas for circular perforation it is about 2870 K. So it can be inferred that for the same inlet conditions, the combustion temperature obtained is higher for star shaped perforation as compared to propellant with circular configuration. High combustion temperature is desired for better combustion

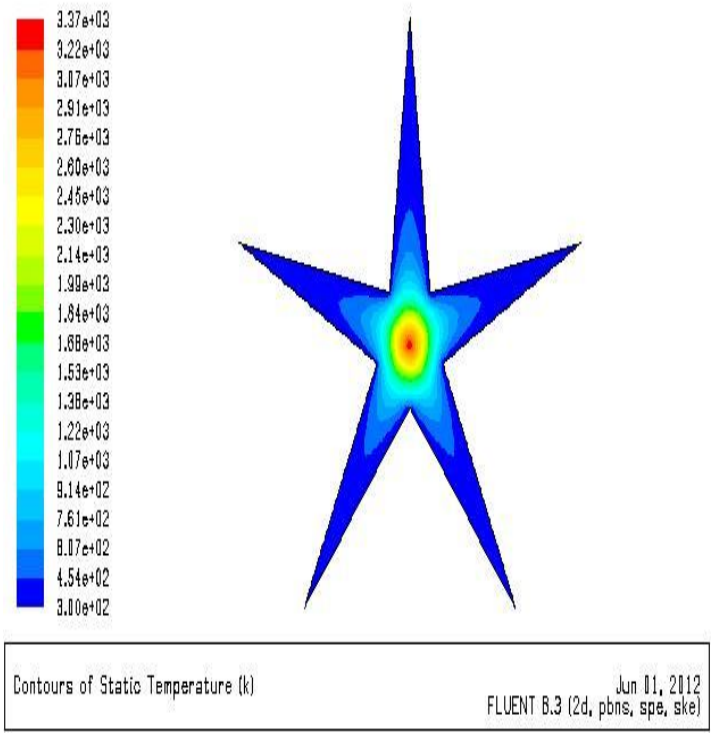

Fig 1: Contours Of Static Temperature Of Five Star Configuration

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

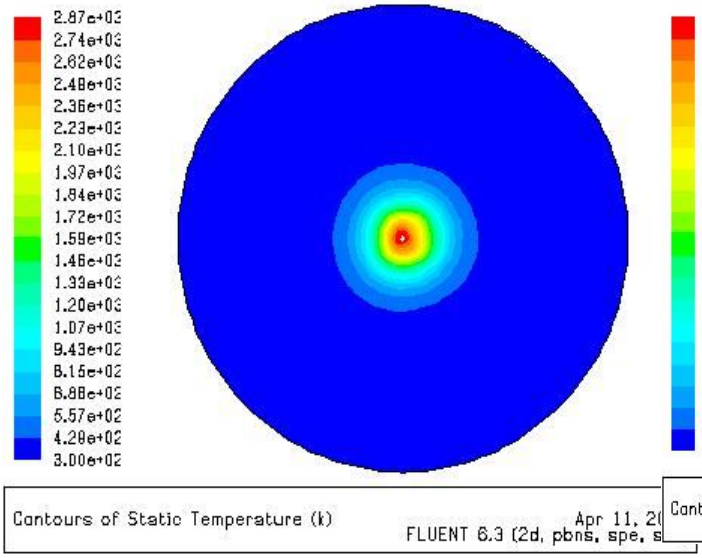

Fig 2: Contours Of Static Temperature Of Circular Perforation

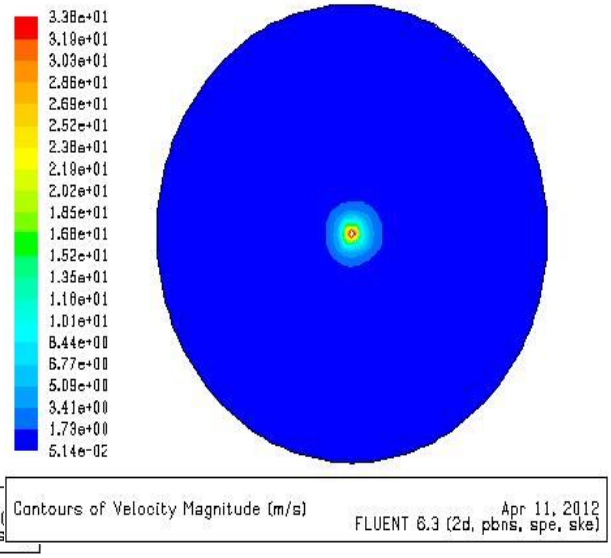

Fig 4:- Contours Of Velocity Magnitude Of Circular Perforation

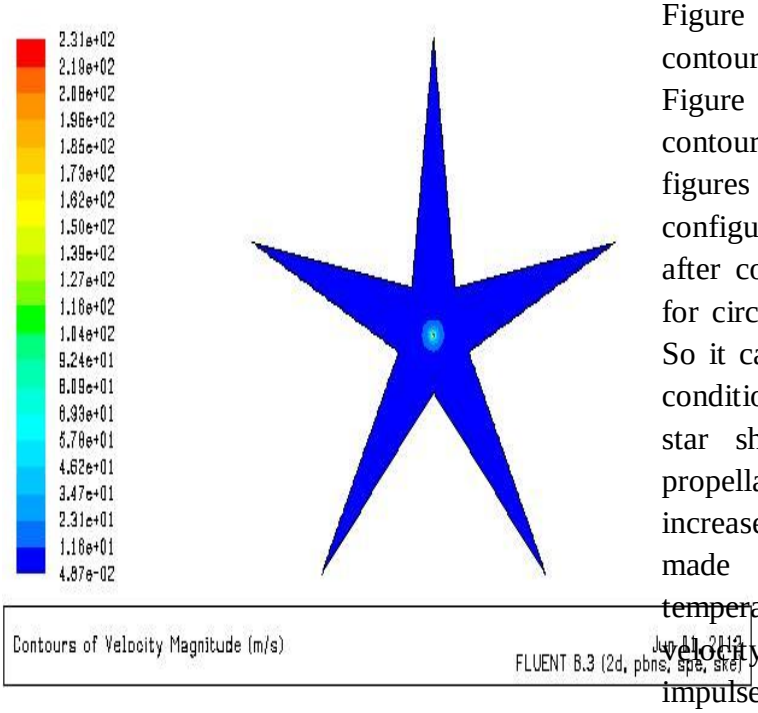

Fig 3: Contours Of Velocity Magnitude Of Five Star Configuration

Figure 3 shows the velocity magnitude contour of the five star configuration and Figure 4 shows the velocity magnitude contour for the circular perforation. From the figures it is clear that for five star configuration, the highest velocity obtained after combustion is about 231 m/s whereas for circular perforation it is about 33.8 m/s. So it can be inferred that for the same inlet conditions, the velocity obtained is higher for star shaped perforation as compared to propellant with circular configuration. The increase in inlet area due to the perforation made is significant as seen from the temperature and velocity contours. High velocity is desired to have more specific impulse for the rocket.

ISSN 2278-3091

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

CONCLUSION

Two dimensional numerical modeling of the combustion zones has been done for ammonium perchlorate composite propellant grain with HTPB binder. Two types of perforations are considered, circular perforation and five leg star configuration or five star configuration. From the velocity and temperature contours it can be found that more temperature and velocity can be generated for the species for star shape configuration than circular perforation because the surface area of burn increases due to the introduction of legs of the star. Although the manufacturing of the star shaped perforation inside the solid grain can be difficult because of the possibility of crack propagation etc., it gives a large advantage over the circular perforation which is easy to manufacture. For better combustion analysis advanced turbulence models can be used for better accuracy. Results obtained from numerical modeling may vary from the experimental data obtained by researchers. It is because of the assumptions considered in this study.

REFERENCES

1. Laredo D. And Gany A., "Combustion Phenomena Of Highly Metallized Solid Propellants", *Acta Astronautica* Vol. 10, No. 5--6, pp. 437-.441, 1~3
2. Ajaz A.G. , Technical Note Estimation of ammonium perchlorate in HTPB based composite solid propellants using Kjeldahl method, Journal Of Hazardous Materials 42 (1995 303- 306)
3. Kaushal Kishore and Kattamachi Sridhara, "Influence of structure of polymeric fuels on the combustion behavior of composite solid propellants", Fuel Vol. 75, No. 7, pp. 912-918, 1996
4. Thakre Piyush and Yang Vigor, "Solid Propellants"
5. AI-Harthi A. and Williams A , "Effect of fuel binder and oxidizer particle diameter on the combustion of ammonium perchlorate based propellants", Fuel Vol. 77, No. 13, pp. 1451-1468, 1998
6. R.P. Fitzgerald and M.Q. Brewster, "Flame and surface structure of laminate propellants with coarse and fine ammonium perchlorate", Combustion and Flame 136 (2004) 313–326
7. Boldyrev V. V, Thermal decomposition of ammonium perchlorate, Thermochimica Acta 443 (2006) 1–36
8. G. Favale, F. Miccio, "Modeling unsteady and perturbed combustion of heterogeneous composite propellants", Aerospace Science and Technology 12 (2008) 285–294
9. Weidong Cai, Piyush Thakre, and Vigor Yang, "A Model Of Ap/Htpb Composite Propellant Combustion In Rocket-Motor Environments", Combust. Sci. and Tech., 180: 2143–2169, 2008
10. S.N. Jawalkar, Mehilal, K. Ramesh, K.K. Radhakrishnan, B. Bhattacharya, "Studies on the effect of plasticiser and addition of toluene diisocyanate at different temperatures in composite propellant formulations", Journal of Hazardous Materials 164 (2009) 549–554
11. Matthew L. Gross, Merrill W. Beckstead, "Diffusion flame calculations for

International Journal of Advanced Trends in Computer Science and Engineering, Vol.2 , No.1, Pages : 235-244 (2013)
Special Issue of ICACSE 2013 - Held on 7-8 January, 2013 in Lords Institute of Engineering and Technology, Hyderabad

composite propellants predicting particle-size effects" Combustion and Flame 157 (2010) 864–873

12. Xiong Gang Wo, Qi-Long Yang, Xin Guo, Xio-Fei Qi, Xaio-Jang Li, K-Qiang Wang [13], "Combustion Efficiency and Pyrochemical Properties of micron-sized metal particles as the components of modified double-base propellant", Acta Astraunautica 2011 1098-1112
13. J. Vandenkerckhove and A. Jaumotte, "Remarks on the Burning Mechanism and Erosive Burning of Ammonium Perchlorate Propellants"
14. J. Powling, "Experiments Relating To The Combustion Of Ammonium Perchlorate Based Propellants"