**SUPPLEMENTATY MATERIAL**

(from References 6 and 7 of the manuscript)

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Numerical Model

## Governing equations

The processes occurring in a hybrid rocket combustion chamber can be adequately described by basic flow equations of continuity, momentum, energy and species. The governing equations which are expressed in 2D axi-symmetric cylindrical co-ordinates are as follows.

*Continuity equation*

 (S.1)

*Axial momentum equation*

 (S.2)

*Radial momentum equation*

(S.3)

 where

*Tangential momentum equation*

 (S.4)

The flow in the combustion chamber and nozzle is likely to be turbulent. Therefore, an appropriate turbulence model is required. The detailed turbulence models like RSM require rigorous closure strategies and grid quality requirements and complexities in computation and convergence1. Hence these are not suited for the parametric study intended here. Simpler models like low-Re *k-ε* turbulence models are widely popular in literature2-5. However, under intense injection the k-ε model fails in qualitative flow prediction6. Although the standard *k-ω* model overcomes this deficiency, it is sensitive to the free stream values of *ω*7. Hence, the SST *k-ω* model was developed8 which combines the advantages of both *k-ε* (free stream accuracy) and standard *k-ω* (near wall accuracy). Thus SST *k-ω* is chosen to predict turbulence in the present study.

The *k equation* is given by

 (S.5)

and the *ω* *equation* is given by

 (S.6)

*Energy equation*

(S.7)

The first three terms on the RHS indicate heat transfer due to conduction, species diffusion and viscous dissipation. The last term is the source term which gives the heat released from the gas phase combustion. *E* and the diffusive mass flux in the above reaction are defined as

 (S.8)

 (S.9)

*Species transport equation*

 (S.10)

Here is the rate of generation or consumption of species *i*

## Gas phase chemistry model

Combustion model with detailed chemistry is desired for accurate predictions. However, proper reaction mechanism and related kinetics are not readily available in the literature. Nevertheless, thermodynamic effect of multi species can be readily incorporated9. Therefore, a global chemistry10 is adopted here where heat of combustion is tuned to be consistent with thermodynamics following ref. 11. This is expected to give reasonable prediction of temperature field and thus heat transfer to the solid fuel. Assuming butadiene as the main pyrolysis product of HTPB, the single step global reaction is given as

(S.11)

According to the law of mass action, the reaction rate *W* is given by assuming a second order reaction as

(S.12)

*k*r can be expressed by Arrhenius law as *k*r=A*exp*(-*E*a/*R*u*T*). Here, A=8.8E+11 and *E*a=1.2637E+08 J/kmol12.

## Solid phase pyrolysis model

The Pyrolysis of the solid fuel (HTPB grain) was modeled by zeroth order Arrhenius equation following ref. 13. The mass of fuel released by pyrolysis is given by

 (S.13)

## Boundary conditions

The boundary types are as mentioned in Fig. 1 of the manuscript. The fuel inlet was defined as an interface where mass and energy balance was applied. The energy balance equation is given by

 (S.14)

The mass balance at the interface is given by

 (S.15)

The convection-diffusion balance equation at the interface is given by,

 (S.16)

Here,

 (S.17)

The equation is solved for *Y*j (the mass fraction of species *j*) on the gas side of interface. Substituting Eq. (S.16) and Eq. (S.17), Eq. (S.14) can be rewritten as,

 (S.18)

The mass balance at the interface is given by,

 (S.19)

The arithmetic sum of the last two terms in Eq. (S.18) gives the heat of pyrolysis of solid fuel. It includes the latent heat of pyrolysis and the arithmetic sum of sensible heats of both solid and gaseous fuel. Thus the Eq. (S.18) becomes

 (S.19)

A part of the thermal energy released in the reaction zone is convected to the solid-gas interface and conducted to the solid fuel (1st term in Eq. (S.19); qconvection). A part of this thermal energy is then transferred into solid fuel by means of conduction in the solid phase (2nd term; qconduction-loss). The remaining energy is utilized for solid fuel pyrolysis (3rd term; qpyrolysis).

The heat lost inside the solid fuel was determined by an analytical solution of 1D heat conduction inside the solid with moving hot boundary. The analytical temperature profile inside the solid fuel is given by

 (S.20)

The radiation heat transfer is neglected in the present study. Simulations2,11 have shown that the effect of radiation (compared to simulations without radiation) on change in net heat flux incident on the solid fuel surface is small (typically about 10%). This is because when radiation is included, the radiation heat flux on the fuel surface increases the blowing velocity which in turn reduces convective-conductive heat flux. Radiation from flame also reduces flame temperature which further reduces convective-conductive heat flux. The net result is only a marginal increase in net heat flux on the fuel surface (or a small increase in regression rate14.

A fixed average mass flux was specified at the oxidizer inlet for both swirling and non-swirling oxidizer flow simulations. Swirl in the inlet was quantified by a non-dimensional parameter called swirl number. It is defined15 as the ratio of axial fluxes of angular momentum to axial momentum, non-dimensionalized by inlet radius.

 (S.21)

The analytical axial and swirl velocity profiles which can be considered as equivalent for swirling flow inlet boundary conditions in CFD are defined15 as

 (S.22a)

 (S.22b)

Substituting these equations in Eq. (S.21) results in the ratio of body force terms *fz* to *fx* as a function of swirl number. Unit magnitude is assumed for *fx* and *fz* was altered to achieve different swirl velocity profiles and thus difference swirl numbers at the inlet. The nozzle was defined as adiabatic walls. Atmospheric pressure was specified at the outlet.

# Validation

## Regression rate calculation

Experiments were carried out in a slab motor2 by Kuo et al. Some of the experiments for which local regression rate was available(test numbers8, 9, 11 and 14) were chosen for model validation.

One major limitation in comparing the prediction from present model to the experiments is in the reporting of regression rates. The experimental values are temporally averaged local regression rate along the axial length of the fuel grain, whereas the simulations performed predict the instantaneous local regression rate. Since the regression rate varies non-linearly with time the averaged value is likely to differ from the predicted value. Further assumption of flat wall will lead to difference in flame stabilization location and hence the local regression rates, especially at the head end. Assumption of global chemistry also limits the prediction of spatial heat release rate in the flame which will effect heat transfer to the fuel and hence the regression rate. Neglecting of radiation in the model is also expected to contribute to mismatch (by about 10%) between experiments and simulations.

Figure 1 (A) represents the schematic of the experimental setup2 used by Chiaverini et al. The upper figure in Fig. 1(B) presents the computation domain used in the initial stage simulations in present validation study. The domain is stretched in y-direction by 3 times for clarity. The computational domain consisted of a 2D combustion chamber and a CD nozzle. The governing equations in cartesian co-ordinates were used in the simulation with the models described in section II. The mesh size used in the combustion chamber was 601 x 76. Grids were clustered towards the fuel surface and inlet to resolve the gradients and the flame stabilization point respectively. The results are discussed in this section.



A B

**Fig. 1 (A) Schematic of experimental set up used by [14], and (B) two dimensional computation domain used for simulations with horizontal fuel grain (upper) and tapered fuel grain (lower)**



A B

**Fig. 2 (A) Validation of present model – Regression rate profile along the axial length of the fuel grain for test no. 11 [ref.** 2**] (B) Comparison of computed regression rate profiles with experiments for test number 8, 9 and 11 of [ref.** 2**]**

Figure 2(A)shows the regression rate profiles predicted by the present model in comparison with the experimental and numerical results2. Initially it was assumed that the port height is uniform throughout the length even though it represented the intermediate case. The regression rate was under predicted in this simulation. The slope of the regression rate did not match the experiments as well. In reality, the fuel surface at the intermediate time would have regressed more at the tail end. It would be appropriate to take that effect into account.

Hence, the computation domain (stretched in y-direction by 3 times for clarity) was modified as shown in lower figure of Fig. 1 (B). The fuel surface was provided an inclination and a post combustion chamber was added. The specification of inclined grain geometry is based on the global regression rate from experiments and the instantaneous spatial regression rate from simulation with straight port at initial port height. The procedure for selecting inclination of regressing surface is explained here. First simulation with horizontal fuel surface at initial port height was performed. It was found that the regression rate at the tail end was three times higher than that at the head end. A linear variation of regression rate from the head end to the tail end was assumed to fix the inclination of the burning surface of the tapered grain. The radial position of this inclined surface was determined such that the average port height matches that of experiments at half burn time. The average port height for experiments was computed by adding twice the product of global regression rate and half burn time to the initial port height.

 Here the predicted regression rate matched well with the experiments over a wide region along the axial length of the motor. In an actual motor, the high regression rate near at the flame stabilization point creates a dent in the fuel surface and the flame gets stabilized at this point. However, a flat fuel surface is used in the simulations where stabilizing the flame becomes difficult. So, the flame is forced to stabilize at the head end by providing a negligible quantity of fuel at fixed temperature at the head end (typically about 0.1% of fuel flow rate). This may be the reason for mismatch near the head end of the motor. In the tail end the actual profile of fuel surface at the entrance of post combustion chamber is not known. This can be the reason for under prediction of the regression rate, yet the steep rise in the regression rate was captured if not accurately. It can be seen from the Fig. 2(A) that the simulation with tapered fuel grain predicts the experiment values much better than the simulation with horizontal fuel grain. Qualitatively the present model captures the regression rate to a very reasonable extent whereas quantitatively the regression rate is under predicted near the head end.

Fig. 2(B) illustrates regression rate profiles along the axial length of the motor for three different experiments2, i.e., experiment numbers 8, 9 and 14. For these experiments also, inclined fuel surface was used. The inclination was based on the inclination of regression rate profile in the initial stage simulation with horizontal fuel surface. It is seen that for experiments 8 and 9, the regression rate trend is predicted reasonably well, whereas for experiment no. 14, there is significant deviation in the upper half of the motor. In experiment no 14, one of the two fuel slabs used was loaded with aluminium particles. This increases heat flux towards the surface by means of radiation which is not accounted for in the present model. With the slabs regressing at different rates, the port variation also will not be symmetric along the centerline. These may be the reasons for such a deviation.

## Swirl flow in a pipe

Steenbergen16 reported experimental measurements on turbulent swirl velocity profiles at various axial locations (x/D = 4.4, 7.6 and 14.5). Since the inlet velocity profile was not known, the reported velocity profile at x/D=4.4 was provided at the inlet in the present simulation. The computed profiles at the sections x/D = 7.6 and 14.5 are compared with the experimental values in Fig. 3. The predicted velocity profiles match well with the measured profiles.



**Fig. 3 A comparison of axial and swirl velocity profiles predicted using present model with the experiments16 in a long cylindrical pipe**

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