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Chemical Kinetics of the TPS and Base Bleeding during Flight Test

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Abstract: The present research deals with thermal degradation of polyurethane foam (PUF) during flight test. Model of thermal decomposition was developed that accounts for polyurethane kinetics parameters extracted from thermogravimetric analyses and radial heat losses to the surrounding environment. The model predicts mass loss of foam, the temperature and kinetic of release of the exhaust gases and char as function of heat and radiation loads. When PUF is heated, urethane bond break into polyol and isocyanate. In the first stage, isocyanate pyrolyses and oxidizes. As a result, the thermo-char and oil droplets (yellow smoke) are released. In the second decomposition stage, pyrolysis and oxidization of liquid polyol occur. Next, the kinetics of chemical compound release and the information about the reactions occurring in the base area are coupled to the CFD simulations of the base flow in a single first stage motor vertically stacked vehicle configuration. The CFD simulations are performed to estimate the contribution of the hot out-gassing, chemical reactions, and char oxidation to the temperature rise of the base flow. The results of simulations are compared with the flight test data.

Keywords: Polyurethane foam, Pyrolysis, Base Heating, and Base Bleeding

1 Introduction

Analysis of the recent test flight data [1] identifies chemically reactive out-gassing as the main root cause for significantly under-predicted temperature rise of the base flow during recent test flight. To include base bleeding effects into CFD simulations of the base flow a model of the conduction and pyrolysis of the thermal protection system materials was developed that predicts surface recession rate, chemical kinetics, composition, temperature, and oxidation rates of the gas and char flow in the base atmosphere.

2 Problem Statement

Foam characterization is carried out by an elementary analysis of the matrix, with the raw chemical formula as $CH_x\ O_y\ N_z$. The chemical formula allows carbon, hydrogen and nitrogen to be balanced between burned mass and gas products. The thermal degradation of polyurethane (PU) can be approximated by a few heterogeneous reactions: pyrolysis and oxidations. The two pyrolysis paths are associated with the main components of PU: polyisocyanate and polyol:

$$n\ OCN\text{-}R\text{-}NCO + HO\text{-}R'\text{-}HO = (R\text{-}NHCOO\text{-}R'\text{-}NHCOO)_n$$

When PU-foam is heated urethane bonds break into polyol and isocianate. Thermo chromatographic analysis of the PU showed that the PU decomposed via a two-steps pyrolysis. In first stage isocyanate pyrolyses and oxidizes. Pyrolysis and oxidization of polyol occur in the second decomposition stage.
Process of decomposition of Polyurethane Froth-Pak (PU) foam under action of radiation and convective heat flux is extremely complex process and the simplest nontrivial model can be presented as three main successive steps:

First pyrolysis and internal oxidation of PU foam begin at 650-860K. This process is endothermic reactions absorbing heat energy. PU pyrolysis results in formation of thermo-char and generation of gas and aerosol of polyurea (yellow smoke). During the first decomposition stage there is formation of gaseous product: hydrocarbon compounds, CO, CO2, HCN and NO.
Secondary pyrolysis begins at 850-1000K molecules of PU continue to crack yielding char and producing flammable gases. During the second stage gaseous compounds containing carbon (CO, CO2) and water characterize the decomposition of polyol. This process is exothermal reactions with heat energy release H_{cT}. Pyrolysis of thermo-char results information of α-char and generation of gas and black smoke.

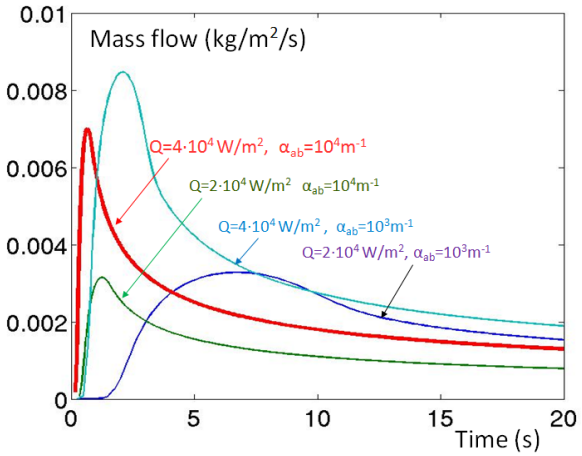

Figure 1: Total gas and char mass flow due to TPS pyrolysis for several radiation flow Q and absorption coefficient.

Third step: char oxidation to secondary char, taking place between 420°C and 570°C. Surface combustion (oxidation) of the α-char layer is exothermal reactions with heat energy release. The reaction rate for the third step reaction is proportional to the oxygen partial pressure.
Density of the all the components is described by continuity equation taking into account their generation or disintegration during the pyrolysis. The temperature was described by the energy equation that took into account the heat released or absorbed by each reaction and a radiation heat from the plume. On the basis of this model the preliminary simulation were done and the gas and char flow and the recession rate were estimated.
Depending on the radiation and the amount of oxygen in the atmosphere the recession rate was 0.2-0.4 mm/s. Fig.1 shows the total mass flow during the pyrolysis of the PU depending on the oxygen partial pressure typical for low and high altitude, the radiation flow and the radiation absorption coefficient α_{ab} that is unknown factor. Radiation was taken from the experimental data. For the low altitude with 20% oxygen atmosphere, radiation Q=4 10^3 W/m^2 and absorption α_{ab} =100 the total mass flow was about 0.035 kg/m^2/s.

3 Conclusion and Future Work

The model was used to estimate the gas and char flow from the TPS of the rocket in the base area. The results were used to simulate base bleeding effect and helped to understand better the experimental results. However the model needs experiments to estimate experimentally unknown parameters. Similar model will be also developed for other TPS materials such as ABL5 cork.

References

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