International Journal of Thermal Sciences 127 (2018) 252–265

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

Thermal conductivity estimation of high solid loading particulate composites: A numerical approach

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ARTICLE INFO

Keywords:
Thermal conductivity
Composites solid propellants
Particulate composite
High solid loading

ABSTRACT

The problem addressed here is the determination of thermal conductivity of high solid loading particulate composites through computational techniques. The primary material of study is a composite solid propellant which is used extensively in the launch vehicle industry and also has application in missiles for the defence sector. Composite propellants generally have a very high solid loading of reinforced particles as compared to the conventional composite materials (particulate composites). Thermal diffusivity is one of the important properties of a propellant which plays a role in determining the thermal profile inside the solid phase of the propellant during its combustion. The thermal profile dictates the energy stored in the condensed phase. The specific heat capacity of the solid and density of the solid depend on the volume, while surface area along with volume could be the controlling parameters in determining thermal conductivity. This study evaluates the thermal conductivity of wide range of composite solid propellants using a numerically developed finite volume model. For this, a simulated propellant pack is constructed using a random packing method, assuming particles as spheres. The results of few of the packs are compared with experiments. The simulations predict a slightly lower value compared to the experimental results probably due to the spherical nature of the particles assumed here. The contact between two particles (spheres) is a point while AP and Al particles are not exactly spherical in nature. As a consequence, the contact surface area is reduced and this reduces the paths of least resistance that could be available for heat flow. The paper brings out the pitfalls of using homogenization of fine sized particles with the matrix.

1. Introduction

Composite materials have found many applications in aerospace industries over the years. Most considerations of composite material usage have been from a structural point of view as composite materials provide high strength, but have less weight as compared to metals, a factor which is crucial in aerospace applications. It must be noted here that most of these class of composite materials have a typical solid loading of additives less than 10% by weight [1] in order to enhance mechanical or thermal properties. However, composite solid propellants used for rocket and missile applications have a high solid loading of up to 87% [2]. The current study is an effort to develop a computational method to predict thermal conductivity of materials with high solid loading such as composite solid propellants.

Composite solid propellants are specialized particulate composite material wherein crystalline Ammonium Perchlorate (AP) particles are mixed in a fuel (also acts as binder) matrix. The fuel considered in this study is Hydroxyl-Terminated Poly-Butadiene (HTPB). Finely powdered Aluminium (Al) is also added to the fuel matrix to enhance the performance. Apart from the fuel and oxidizer there are small quantities of plasticizer, curative agent and other additives. Sometimes iron oxide (IO) and copper chromite (CC) are also added as burn rate enhancers.

One critical parameter of propellant performance is the burn rate which depends on various factors like propellant composition, pressure and initial temperature. The burn rate of the solid propellant as the function of chamber pressure and initial temperature for a given composition is shown in Eq. (1) [2,3].

$$\dot{r} = aP_C^n \tag{1}$$

$$a = a_o e^{\sigma_P (T_{in} - T_0)} \tag{2}$$

where, P_C = Chamber pressure, (in Pascal), a = Burn rate of solid propellant at unit pressure, m/s, n = burn rate pressure index, σ_P = temperature sensitivity, $\%/K$. a_o and T_0 are the burn rate at unit pressure and temperature at standard conditions. T_{in} is the initial temperature of the propellant.

Ishitha and Ramkrishna [4] have shown a strong relationship between the burn rate pressure index and the thermal conductivity of the

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https://doi.org/10.1016/j.ijthermalsci.2018.01.023
Received 27 June 2017; Received in revised form 8 November 2017; Accepted 18 January 2018

Nomenclature

α_{AP}	Thermal diffusivity of AP, m^2/s
α_{HTPB}	Thermal diffusivity of HTPB, m^2/s
$\dot{r}$	Burn rate, m/s
$\lambda_{i,j,m}$	Interface thermal conductivity for cell (i, j, m) in x-direction, W/mK
ϕ	Volumetric packing fraction
ρ	Density, kg/m^3
ρ_n	Density of constituent n, kg/m^3
σ_P	Temperature Sensitivity, $\%/K$
A	Cross sectional area of YZ plane in cubical domain, m^2
a	Burn rate of solid propellant at unit pressure, m/s
a_0	Burn rate of solid propellant at unit pressure under standard condition, m/s
A_{cell}	Interface area for cell, m^2
a_{nb}	Temperature coefficient for the neighbouring point of P, W/K
a_P	Temperature coefficient for temperature at point P at present time step, W/K
a_P^0	Temperature coefficient for temperature at point P at previous time step, W/K
B_i	Biot number
$C_{p,n}$	Specific heat of constituent n, J/kgK
C_p	Specific heat in condensed phase, J/kgK
d	Particle diameter, m
e_v	Volumetric error in capturing the single particle in cartesian grid
i, j, m	Grid centre location in cartesian coordinates
k	Thermal conductivity, W/mK
k_{AP}	Thermal conductivity of AP particle, W/mK
k_{eff}	Effective Thermal conductivity in condensed phase, W/mK
k_f	Thermal conductivity of filler particle in composite propellant pack, W/mK
k_{HTPB}	Thermal conductivity of HTPB, W/mK
$k_{i,j,m}$	Thermal conductivity assigned to grid cell $P_{i,j,m}$, W/mK
k_m	Thermal conductivity of matrix material in composite propellant pack, W/mK
k_P	Thermal conductivity assigned at grid centre P, W/mK
$L_x, L_y, L_z = L$	Length of the cubical domain in x,y and z directions respectively, m
M_P	Total mass of the propellant pack, kg
N	No. of cells in each direction
n	Constituent in composite propellant pack
n_c	Number of constituents in composite propellant pack
n_g	Number of grid cells assigned as the particle properties
P_C	Chamber pressure, Pa
$P_{i,j,m}$	Grid centre located at (i, j, m) in the domain
Q	Overall heat flow rate through the cubical domain in x-direction, W
q	Overall Heat flux through the cubical domain in x-direction, W/m^2
$Q_{i,j,m}$	Heat flow rate from grid cell $P_{i,j,m}$ to $P_{i+1,j,m}$, W
Q_i	Overall heat flow rate from plane at $x = i$ to $x = i + 1$ in the cubical domain, W
q_i	Heat flux from plane at $x = i$ to $x = i + 1$ in the cubical domain, W/m^2
r	Particle radius, m
R_{int}	Inter-facial thermal resistance, K/W
R_P	Residue in temperature value at grid cell P
T	Temperature, K
t	Time step, s
T^0	Temperature at standard condition, K
T_P^0	Temperature at grid cell P at previous time-step, K
T^1	Initial temperature at which burn rate is calculated, K
$, T_2$	Temperature on the surface at $x = 0$ and $x = L_x$ of cubical domain respectively, K
$T_{i,j,m}$	Temperature at grid cell centre $P_{i,j,m}$, K
T_{nb}	Temperature at neighbouring points of grid cell P, K
V	Total volume of cubical domain, m^3
V_a	Actual volume of particle, m^3
V_c	Captured volume of single particle in cartesian grid, m^3
v_g	Volume of the single grid cell, m^3
V_n	Volume of constituent n in cubical domain, m^3
x, y, z	Cartesian coordinates
$\Delta x, \Delta y, \Delta z$	Grid size in x, y and z direction respectively, m

solid propellant. They observed a decrease in burn rate pressure index with decrease in thermal conductivity.

Gaurav and Ramakrishna [5] have also argued that thermal diffusivity of the propellant plays a role in determining the temperature and pressure sensitivity of the composite solid propellant. They argue that the thermal profile in the propellant depends on the thermal diffusivity, which in turn dictates the energy stored in the condensed phase. The propellants with higher thermal diffusivity have a large penetration depth and these are seen to have higher temperature sensitivity too.

In composite solid propellants, the ingredients are nearly in the same ratio and particle sizes are varied to obtain different ballistic properties. Thus, one would expect the density and the specific heat capacity do not change as they are dependent on the volume. It is only the thermal conductivity which depends on surface area of contact to change in these compositions. Thus, it is important to be able to predict the thermal conductivity of the propellant based on its particle size distribution.

The thermal conductivity of a composite material depends on the thermal conductivity of the constitutive components as stated by Progelhof et al. [6]. Evaluating the effective thermal conductivity correctly will lead to accurate prediction of burning behaviour. Literature reveals that several studies have been carried out to predict the effective thermal conductivity of the composite solid propellant. Effective thermal conductivity of composites has been estimated by Maxwell [7], who gives an analytic expression to determine the same for very dilute dispersion of particles given as.

$$k_{eff} = \frac{k_f + 2k_m + 2\phi(k_f - k_m)}{k_f + 2k_m - \phi(k_f - k_m)}.\ k_m \tag{3}$$

where, k_f, k_m = thermal conductivity of filler (particle) and matrix respectively, ϕ = volumetric loading fraction. The thermal interaction between the particles is not considered here and the formula is valid only for lower values of ϕ limited upto 25 %. After him, several modifications were made to the expression proposed. A good review of this class of work can be found in Pietrak et al. [8]. Chen et al. [9] proposed homogenization of a numerically constructed propellant with the assumption that the small scale particles are homogenized with the binder. The assumption made for homogenization is such that it is possible when their individual thermal conductivities do not differ much. However, there is a difference between the thermal conductivities of AP and matrix. Moreover, the difference is extremely large when other constituents like Al, IO and CC are considered, as noted by Zannoti et al. [10]. Also, thermal conductivity was shown to be a function of the ratio of thermal conductivities of oxidizer and binder and the volumetric loading. However, Gaurav and Ramakrishna [5] have carried out experiments in which they observed a variation in thermal conductivity when they used different particle sizes of aluminium keeping volumetric loading same in both cases.

Devpura et al. [11,12] have predicted the effective thermal